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Scientific and Technical Information Center

SEARCH REQUEST FORM

Requester's Full Name: Jon Eric Angell Examiner #: 78697 Date: 6-14-05
Art Unit: 1635 Phone Number: 2-8756 Serial Number: 09/666,144
Location (Bldg/Room#): REM2020 (Mailbox #): R2218 Results Format Preferred (circle): PAPER DISK

To ensure an efficient and quality search, please attach a copy of the cover sheet, claims, and abstract or fill out the following:

Title of Invention: Chiral, charged peptide nucleic acid oligomers for gene
Inventors (please provide full names): KUMAR et al.

Earliest Priority Date: 9-20-2000

Search Topic:

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known.

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

Please search the formula of claim 14, 15, 19

as well as compounds (4a) and (6a) of claim 20

Please feel free to contact me if you have any questions

Thank you.
Eric

Note: Claims listing is attached

Best Available Copy

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Searcher Location: _____	____ Structure (#)	____ Westlaw ____ WWW/Internet
Date Searcher Picked Up: _____	____ Bibliographic	____ In-house sequence systems
Date Completed: _____	____ Litigation	____ Commercial ____ Oligomer ____ Score/Length
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=> fil reg

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STRUCTURE FILE UPDATES: 11 JUL 2005 HIGHEST RN 854584-06-8
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* The CA roles and document type information have been removed from *
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*

Crossover limits have been increased. See HELP CROSSOVER for details.

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FILE COVERS 1907 - 12 Jul 2005 VOL 143 ISS 3
FILE LAST UPDATED: 11 Jul 2005 (20050711/ED)

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This file contains CAS Registry Numbers for easy and accurate

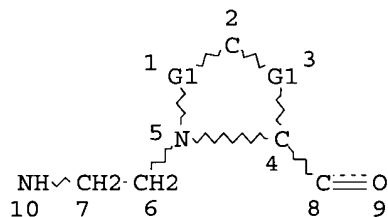
substance identification.

=> s 137

L38 11 L33 OR L36 OR L24

=> d que

L11 STR



REP G1=(1-2) CH2

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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

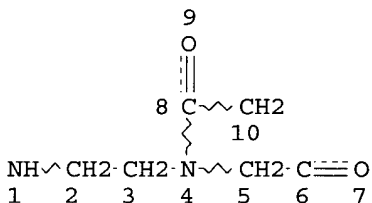
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STEREO ATTRIBUTES: NONE

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L14 2 SEA FILE=REGISTRY ABB=ON PLU=ON L13 AND PMS/CI

L16 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE

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L19 26 SEA FILE=REGISTRY ABB=ON PLU=ON L18 AND L13

L20 3 SEA FILE=HCAPLUS ABB=ON PLU=ON L19

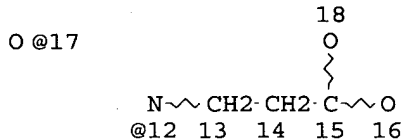
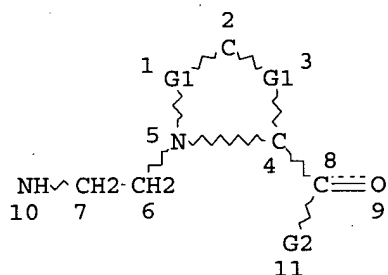
L21 6 SEA FILE=HCAPLUS ABB=ON PLU=ON L13 AND L18

L22 6 SEA FILE=HCAPLUS ABB=ON PLU=ON L20 OR L21

L23 1 SEA FILE=HCAPLUS ABB=ON PLU=ON L14

L24 7 SEA FILE=HCAPLUS ABB=ON PLU=ON L22 OR L23

L29 STR

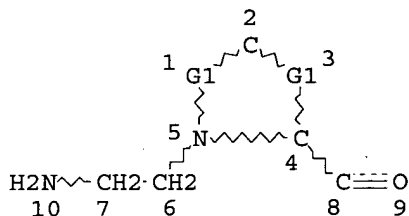


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 CONNECT IS E1 RC AT 16
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 GGCAT IS LIN LOC SAT AT 20
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 DEFAULT ECLEVEL IS LIMITED

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 NUMBER OF NODES IS 25

STEREO ATTRIBUTES: NONE
 L30 46 SEA FILE=REGISTRY SUB=L13 SSS FUL L29
 L31 STR



REP G1=(1-2) CH2
 NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE

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 L33 8 SEA FILE=HCAPLUS ABB=ON PLU=ON L30 AND L32
 L34 14106 SEA FILE=HCAPLUS ABB=ON PLU=ON BIOTIN+PFT,NT/CT
 L35 24339 SEA FILE=HCAPLUS ABB=ON PLU=ON FLUORESCENT SUBSTANCES+PFT,NT/
 CT
 L36 2 SEA FILE=HCAPLUS ABB=ON PLU=ON L30 AND (L34 OR L35 OR BIOTIN
 OR FLUORES? OR FLUOROPHOR?)
 L38 11 SEA FILE=HCAPLUS ABB=ON PLU=ON L33 OR L36 OR L24

=> d l38 ibib abs hitind hitstr 1-11

L38 ANSWER 1 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:769359 HCAPLUS

DOCUMENT NUMBER: 142:38511

TITLE: (2S,5R/2R,5S)-Aminoethylpipercolyl aepip-aegPNA

chimera: synthesis and duplex/triplex stability

AUTHOR(S): Shirude, Pravin S.; Kumar, Vaijayanti A.; Ganesh, Krishna N.

CORPORATE SOURCE: Division of Organic Chemistry (Synthesis), National Chemical Laboratory, Pune, Maharashtra, 411008, India

SOURCE: Tetrahedron (2004), 60(42), 9485-9491

CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB This article reports the design and facile synthesis of novel chiral six-membered PNA analogs (2S,5R/2R,5S)-1-(N-Boc-aminoethyl)-5-(thymine-1-yl)pipercolic acid, aepipPNA IV, that upon incorporation into standard aegPNA sequences effected stabilization of complexes with complementary target DNA. Substitution of aegPNA unit by the designed monomer at the C-terminus was more effective than substitution at N-terminus. The stabilizing behavior improved with degree of substitution and was found to be dependent on their relative positions in the sequence. The six-membered piperidine ring in the design may freeze the rigid chair conformations and the relative stereochem. of the substituents may in effect direct the complex formation with DNA/RNA by sequence-specific nucleobase recognition. In the present aepipPNA analogs, the L-trans stereochem. disposition of the substituents seems to lead to the favorable pre-organization of the PNA oligomers for complex formation with DNA. The results reported here further expand the repertoire of cyclic PNA analogs.

CC 34-3 (Amino Acids, Peptides, and Proteins)

Section cross-reference(s): 6, 33

IT 695183-80-3P 695183-82-5P 797801-67-3P

801322-94-1P 801322-95-2P 801322-96-3P 801322-97-4P 801322-98-5P

801322-99-6P 801323-00-2P 801323-01-3P 801323-02-4P 801323-03-5P

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802988-11-0P 802988-12-1P 802988-13-2P 804568-66-9P 804568-67-0P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(synthesis and duplex/triplex stability of (2S,5R/2R,5S)-

aminoethylpipercolyl aepip-aegPNA chimera)

IT 56-86-0, L-Glutamic acid, reactions 617-65-2, Glutamic acid 4330-20-5, n3 Benzoylthymine 30525-89-4, Paraformaldehyde 96628-67-0

139166-80-6 729601-87-0 801322-92-9 801322-93-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(synthesis and duplex/triplex stability of (2S,5R/2R,5S)-

aminoethylpipercolyl aepip-aegPNA chimera)

IT 5619-01-2P 6893-26-1P, D-Glutamic acid 19525-56-5P 117836-26-7P

150823-40-8P 189952-46-3P 253307-86-7P 695183-56-3P
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 695183-73-4P 695183-75-6P 797801-60-6P 797801-61-7P
 797801-62-8P 797801-63-9P 797801-64-0P
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RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis and duplex/triplex stability of (2S,5R/2R,5S)-aminoethylpipecolyl aepip-aegPNA chimera)

IT 695183-80-3P 695183-82-5P 797801-67-3P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (synthesis and duplex/triplex stability of (2S,5R/2R,5S)-aminoethylpipecolyl aepip-aegPNA chimera)

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CN Adenosine, 2'-deoxyadenylyl-(3'→5')-2'-deoxyadenylyl-(3'→5')-2'-deoxyadenylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxyadenylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxyadenylyl-(3'→5')-2'-deoxy-, complex with peptide nucleic acid ([[(2S,5R)-1-(2-aminoethyl)-5-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-2-piperidinyl]carbonyl]-T-C-T-C-T-T-T)-Bal-OH (1:2) (9CI) (CA INDEX NAME)

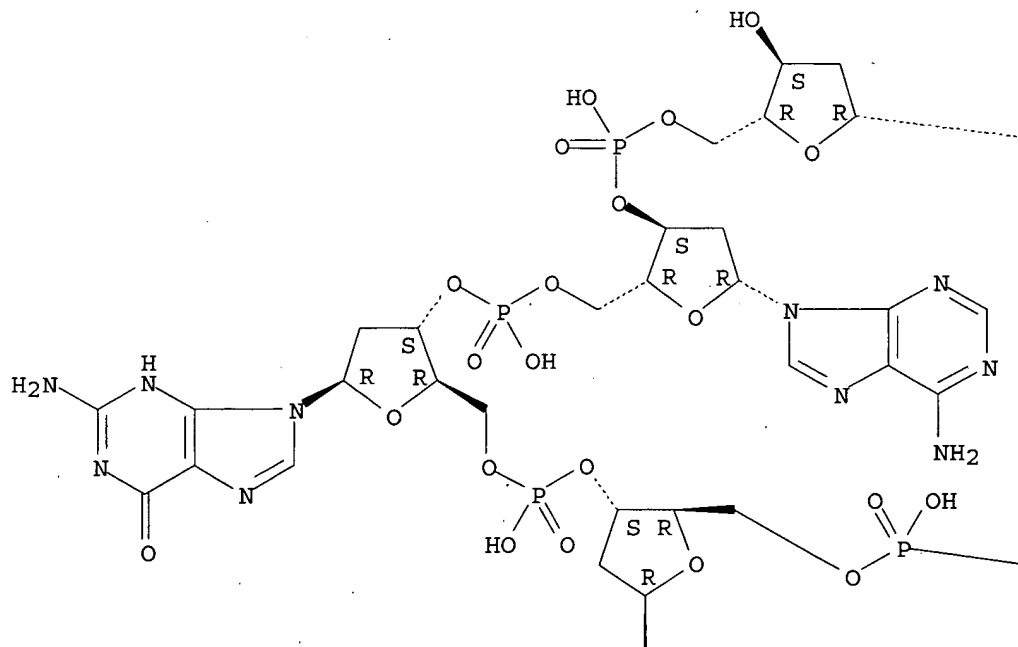
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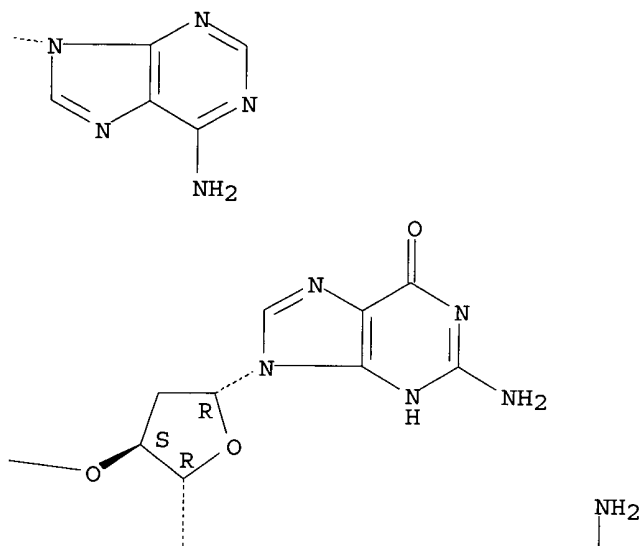
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Absolute stereochemistry.

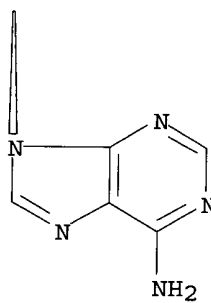
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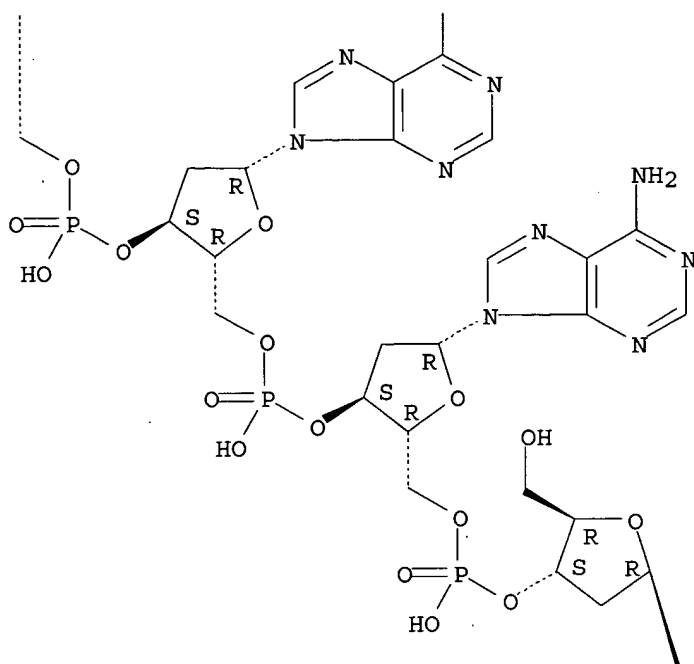
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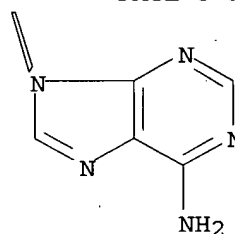
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PAGE 2-B



PAGE 3-B



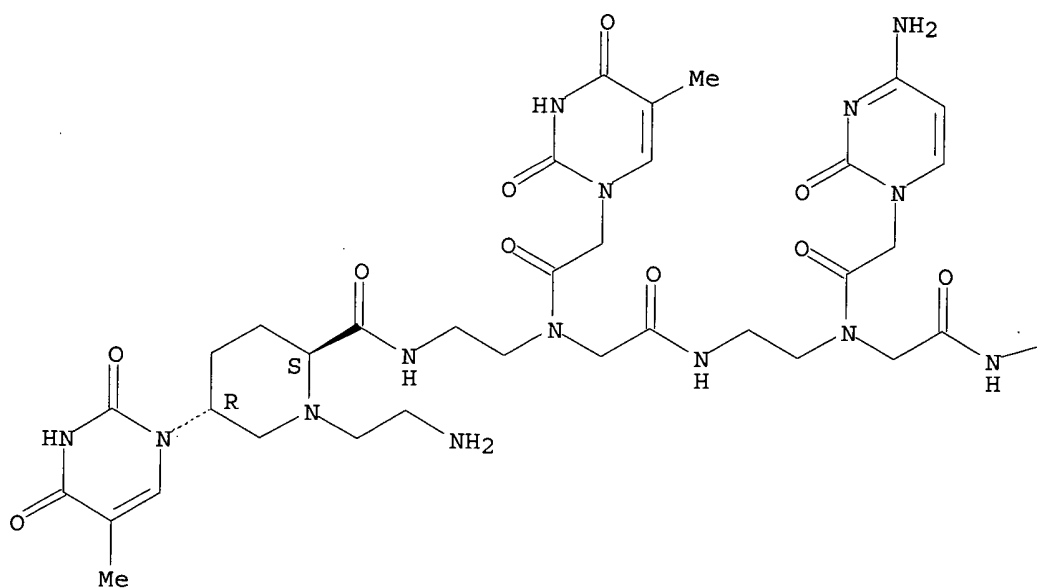
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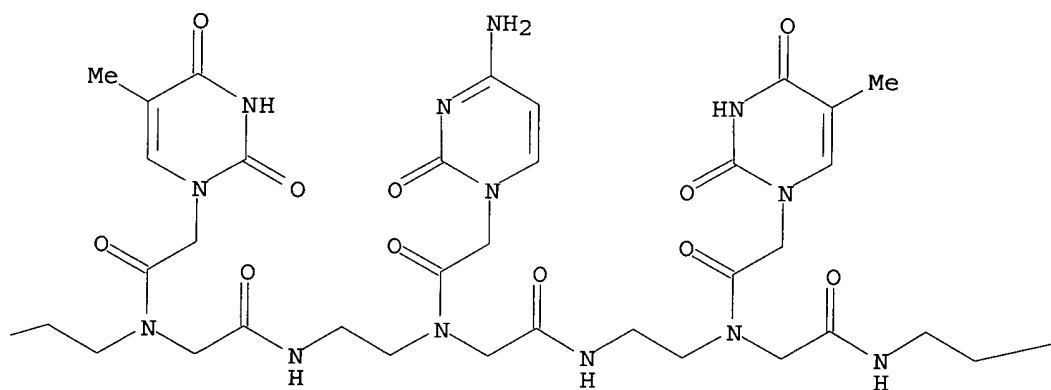
CMF C91 H121 N35 O31

Absolute stereochemistry.

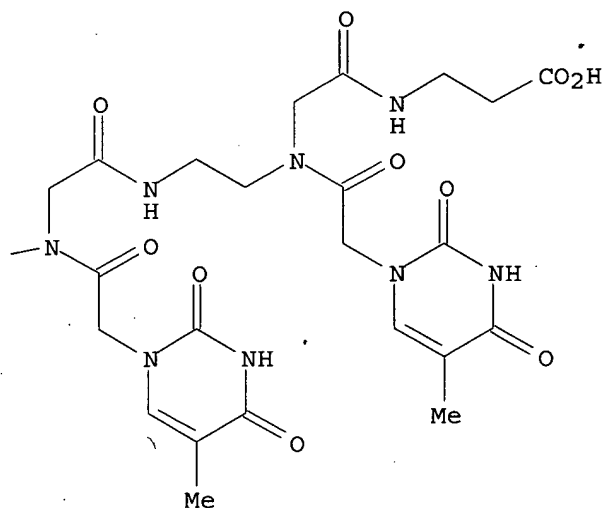
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PAGE 1-B



PAGE 1-C



RN 695183-82-5 HCAPLUS

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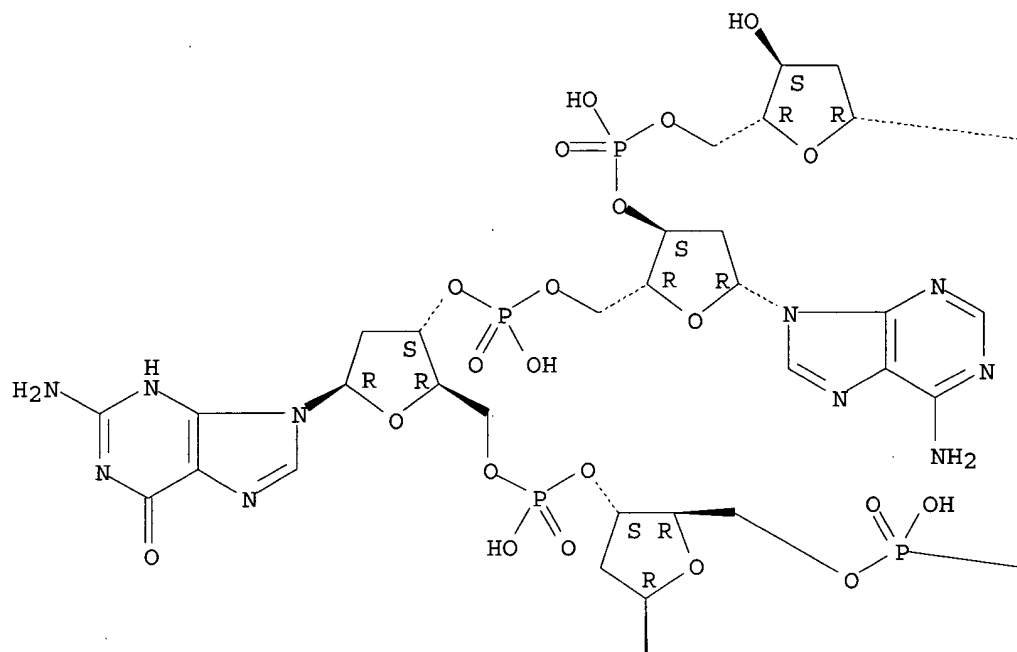
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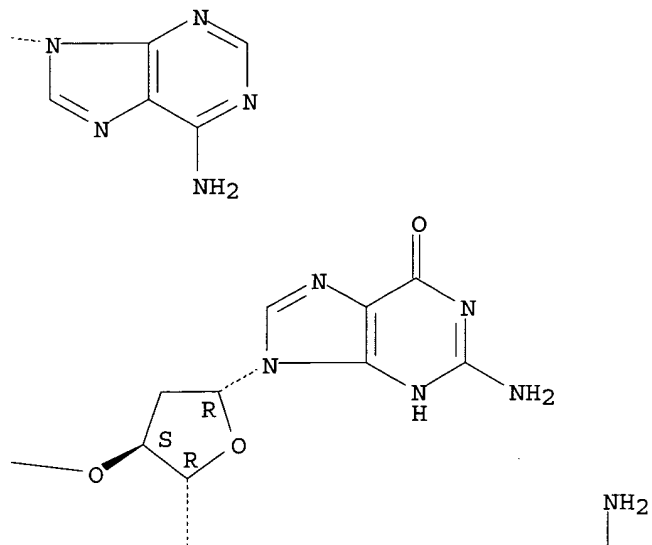
CMF C80 H97 N40 O40 P7

Absolute stereochemistry.

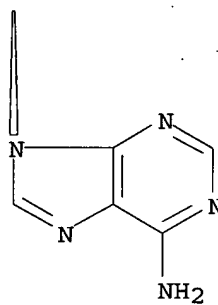
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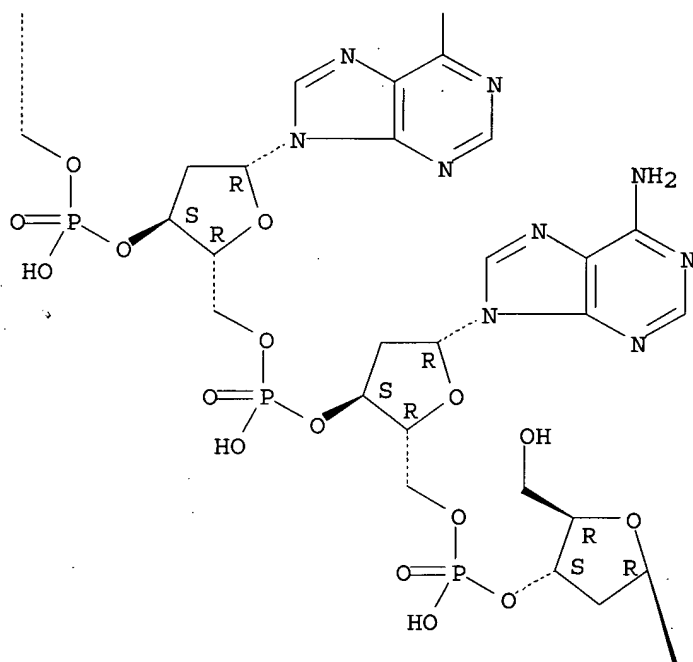
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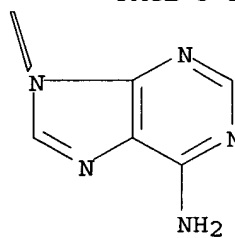
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PAGE 2-B

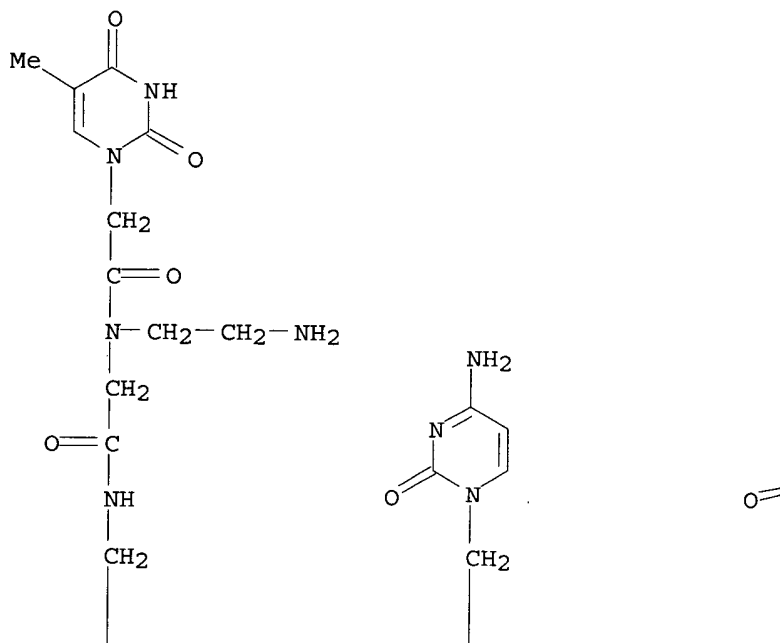


PAGE 3-B

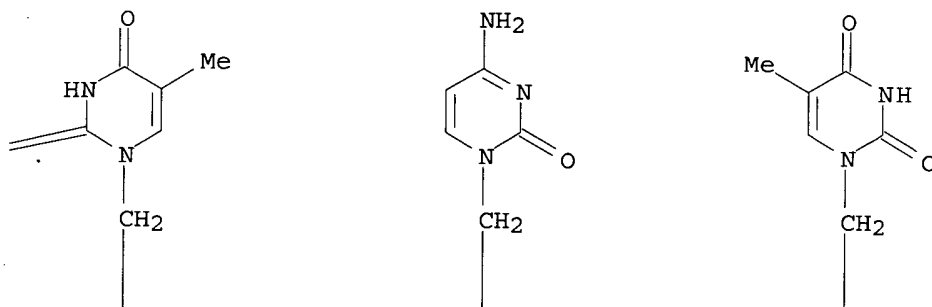


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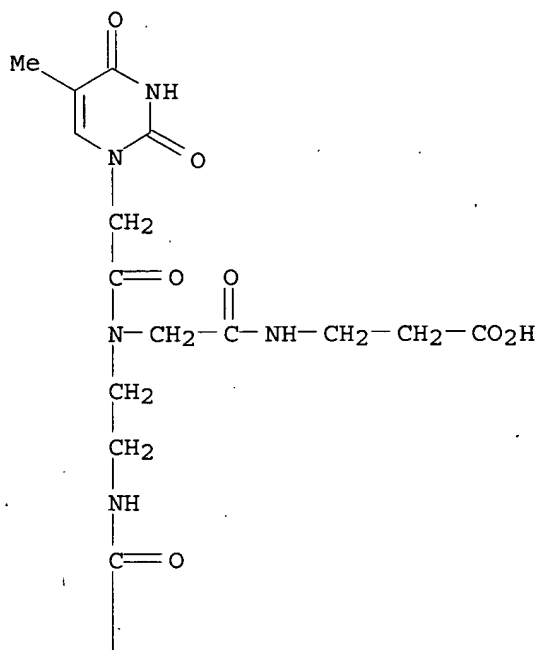
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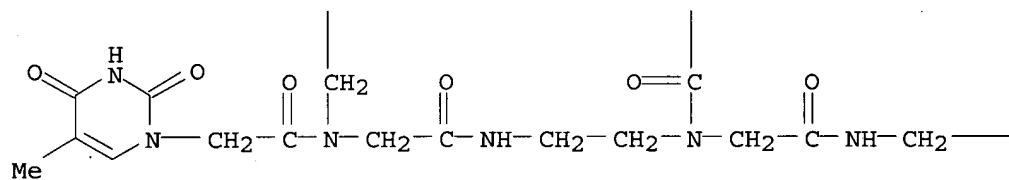
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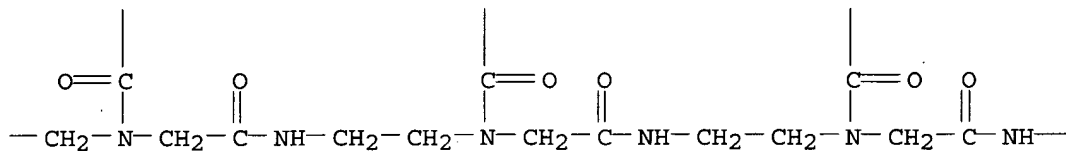
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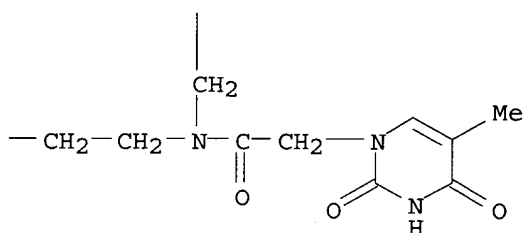
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PAGE 2-B



PAGE 2-C



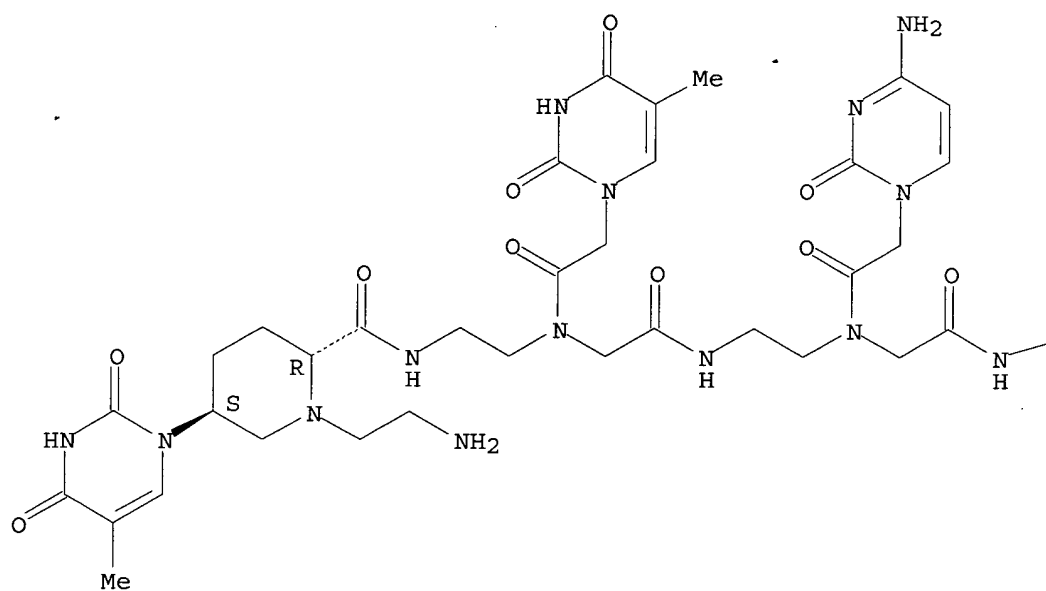
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CM 1

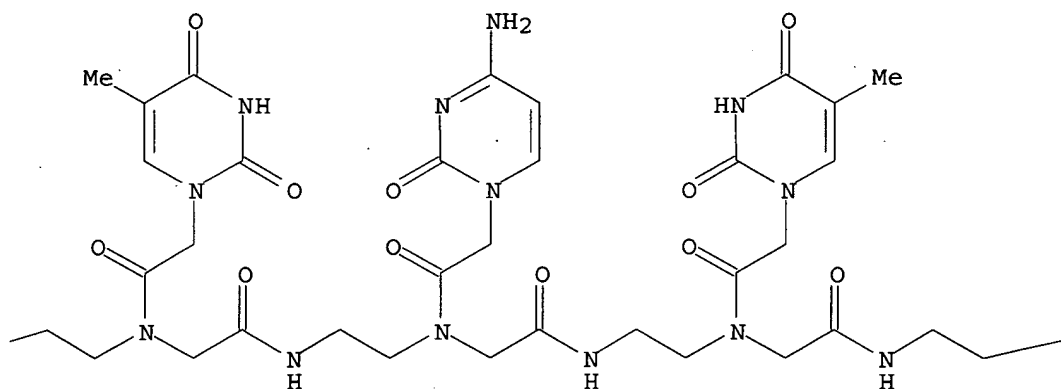
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Absolute stereochemistry.

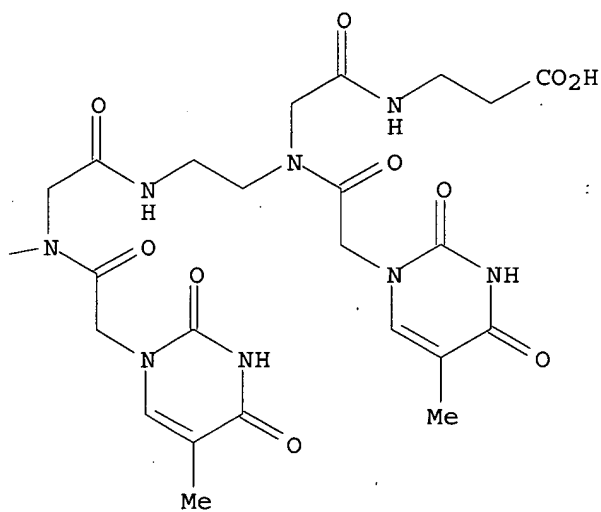
PAGE 1-A



PAGE 1-B



PAGE 1-C



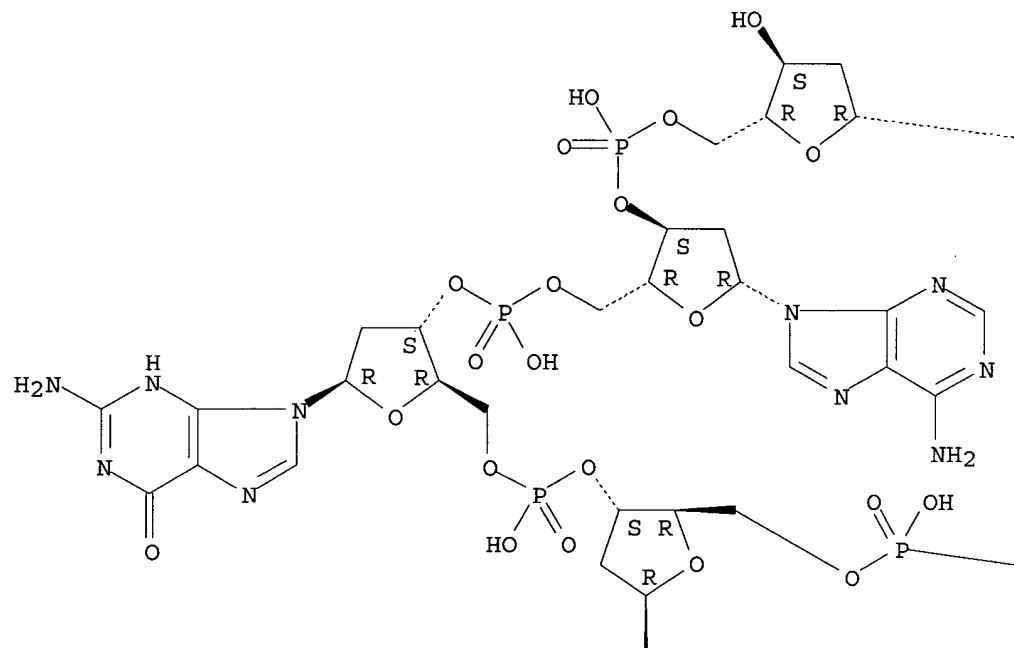
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CRN 695183-78-9

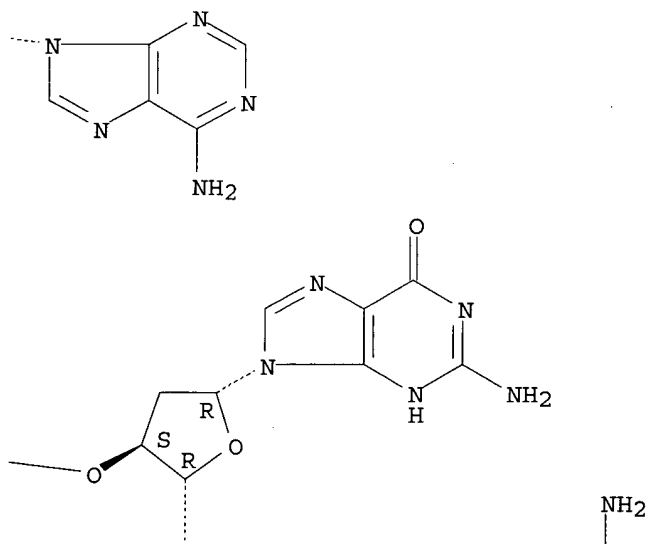
CMF C80 H97 N40 O40 P7

Absolute stereochemistry.

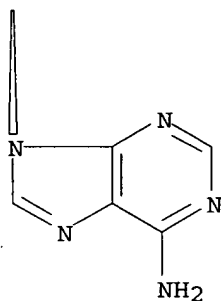
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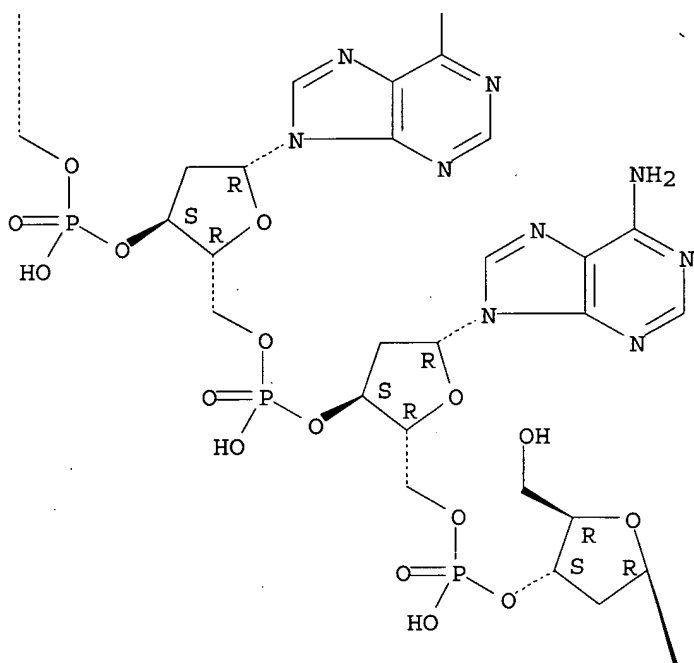
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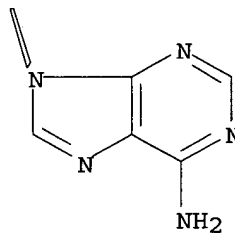
PAGE 2-A



PAGE 2-B



PAGE 3-B



IT 139166-80-6 729601-87-0

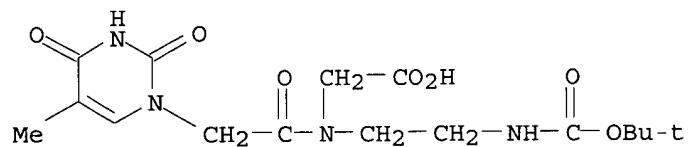
RL: RCT (Reactant); RACT (Reactant or reagent)

(synthesis and duplex/triplex stability of (2S,5R/2R,5S) -

aminoethylpipecolyl aepip-aegPNA chimera)

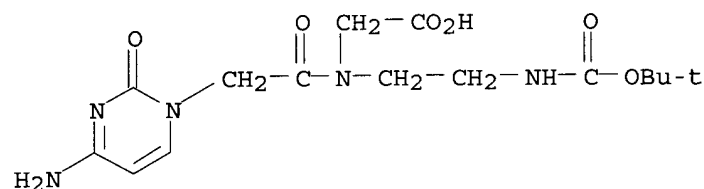
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CN Glycine, N-[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-N-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]- (9CI) (CA INDEX NAME)



RN 729601-87-0 HCAPLUS

CN Glycine, N-[(4-amino-2-oxo-1(2H)-pyrimidinyl)acetyl]-N-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]- (9CI) (CA INDEX NAME)



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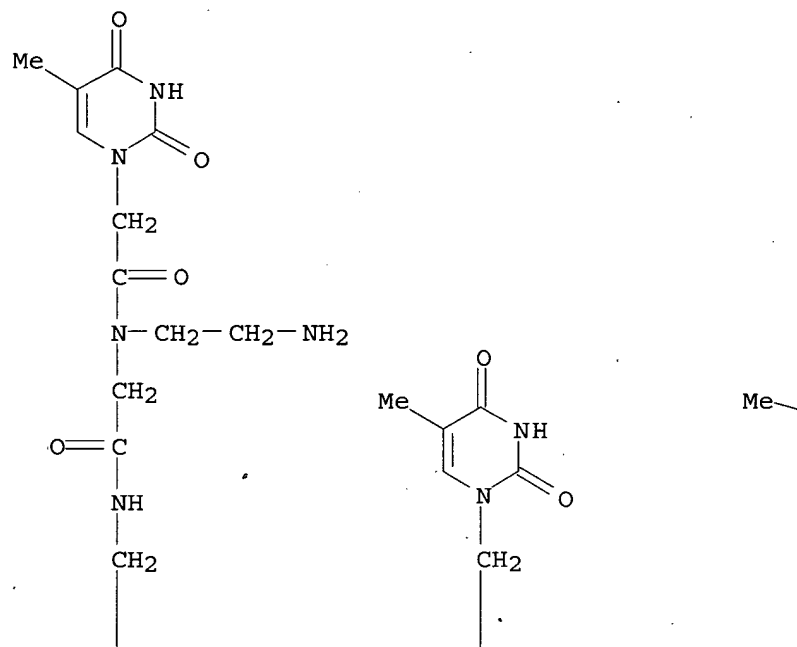
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)

(synthesis and duplex/triplex stability of (2S,5R/2R,5S)-
 aminoethylpipecolyl aepip-aegPNA chimera)

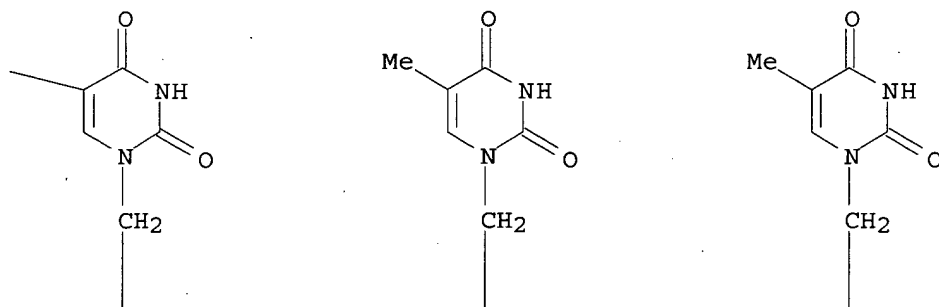
RN 253307-86-7 HCAPLUS

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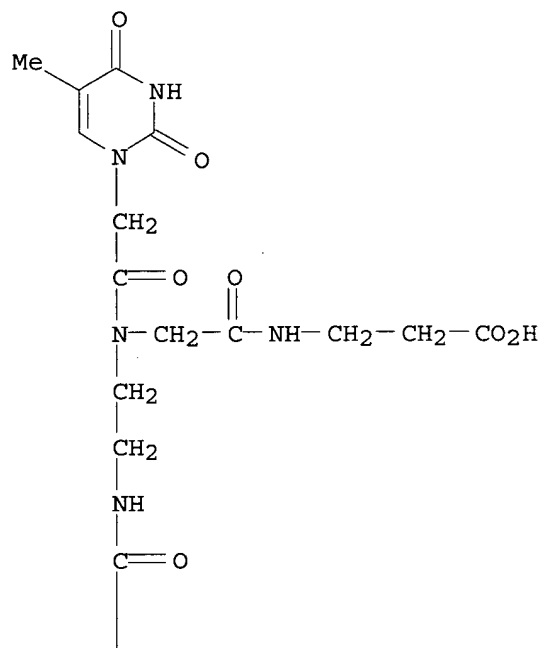
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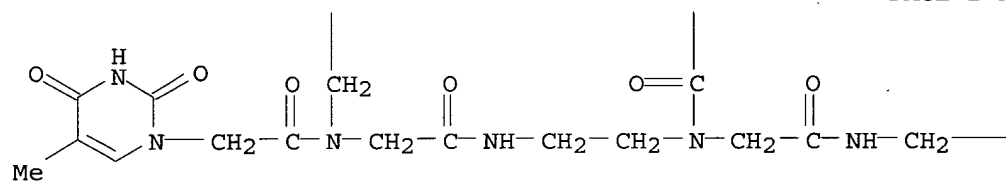
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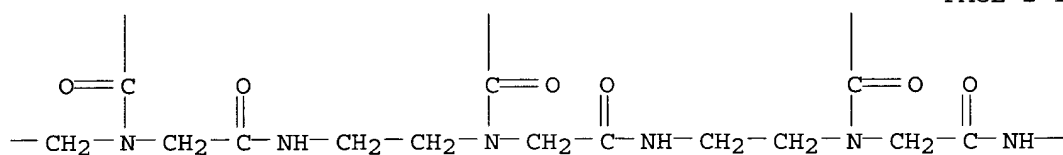
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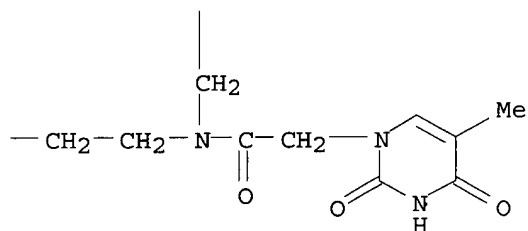
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PAGE 2-B



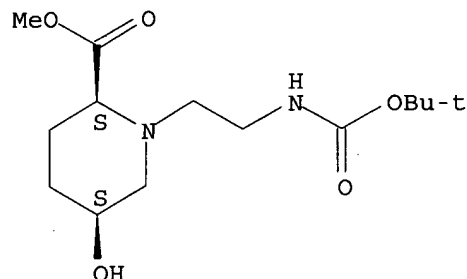
PAGE 2-C



RN 695183-56-3 HCAPLUS

CN 2-Piperidinecarboxylic acid, 1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-5-hydroxy-, methyl ester, (2S,5S)- (9CI) (CA INDEX NAME)

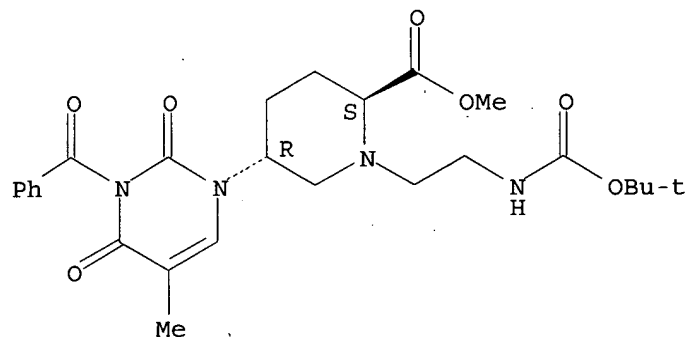
Absolute stereochemistry. Rotation (-).



RN 695183-59-6 HCAPLUS

CN 2-Piperidinecarboxylic acid, 5-(3-benzoyl-3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, methyl ester, (2S,5R)- (9CI) (CA INDEX NAME)

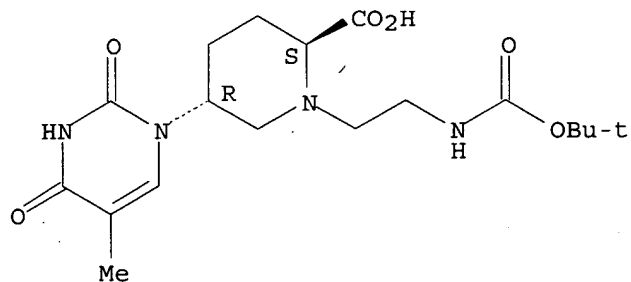
Absolute stereochemistry. Rotation (+).



RN 695183-62-1 HCAPLUS

CN 2-Piperidinecarboxylic acid, 5-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, (2S,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

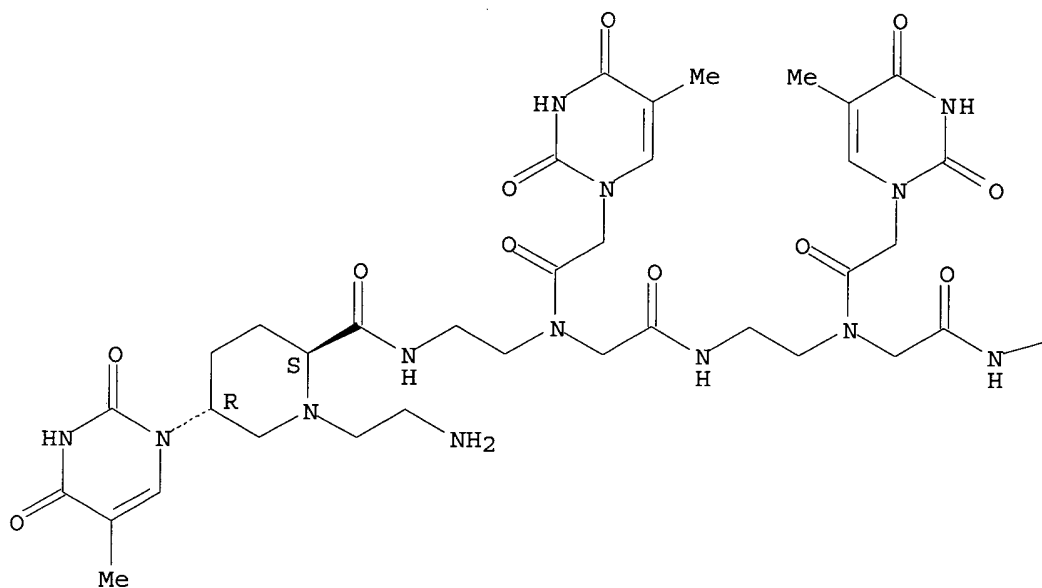


RN 695183-64-3 HCAPLUS

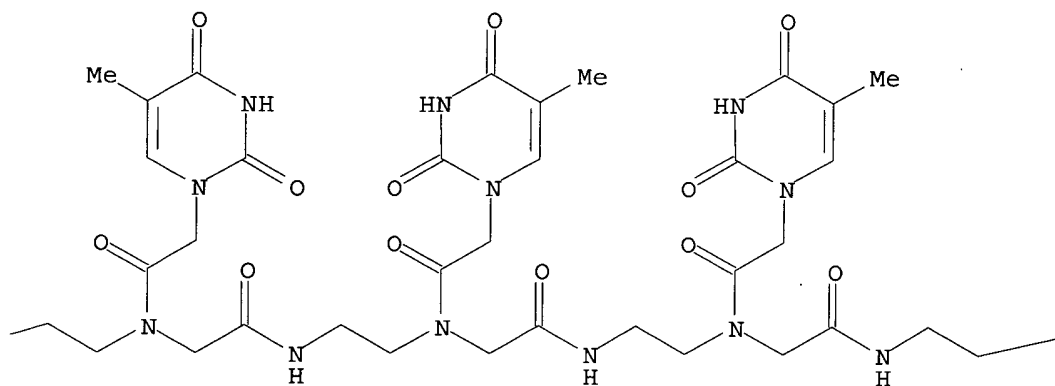
CN Peptide nucleic acid, ([[2S,5R)-1-(2-aminoethyl)-5-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-2-piperidinyl]carbonyl]-T-T-T-T-T-T)-Bal-OH (9CI) (CA INDEX NAME)

Absolute stereochemistry.

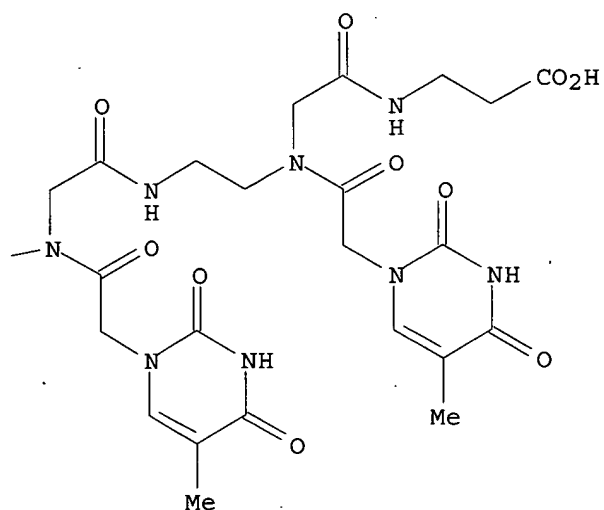
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PAGE 1-B



PAGE 1-C

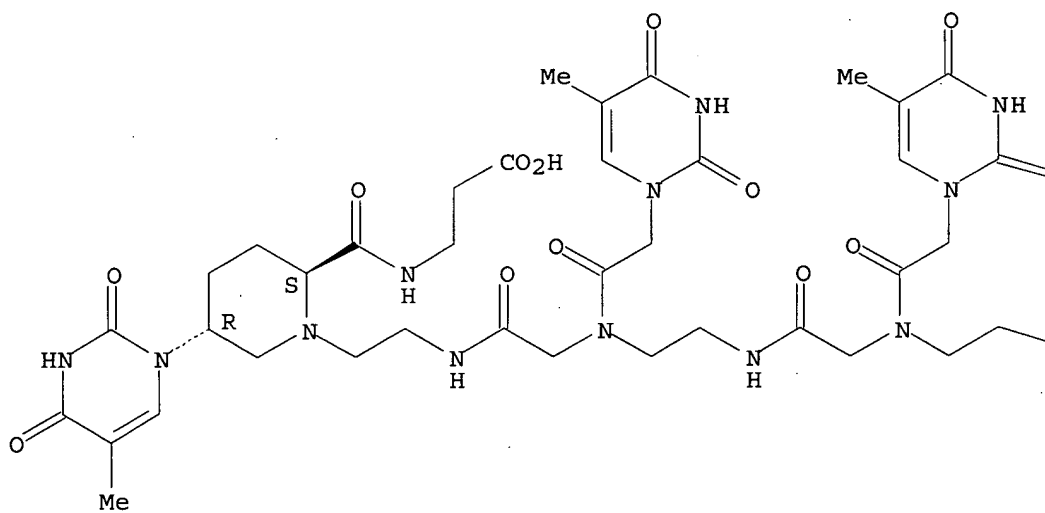


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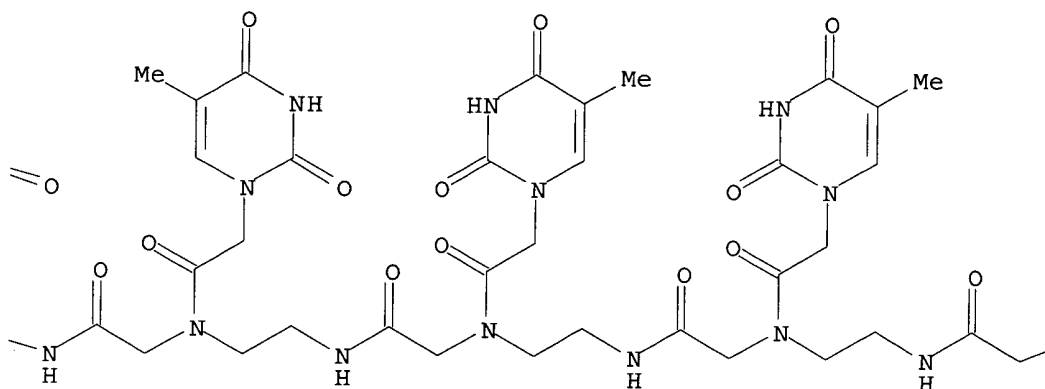
CN Peptide nucleic acid, (H-T-T-T-T-T-T-T)-(2S,5R)-1-(2-aminoethyl)-5-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pip-Bal-OH (9CI) (CA INDEX NAME)

Absolute stereochemistry.

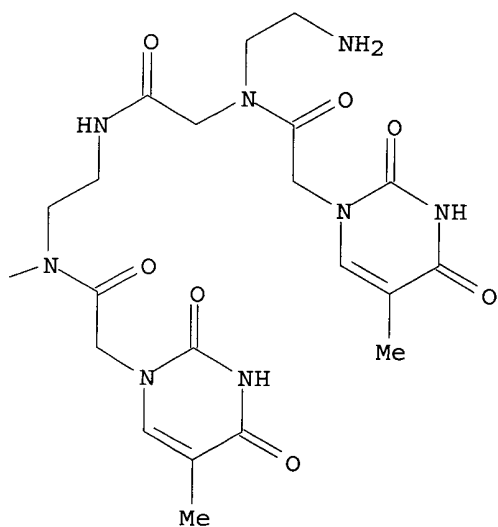
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PAGE 1-B



PAGE 1-C

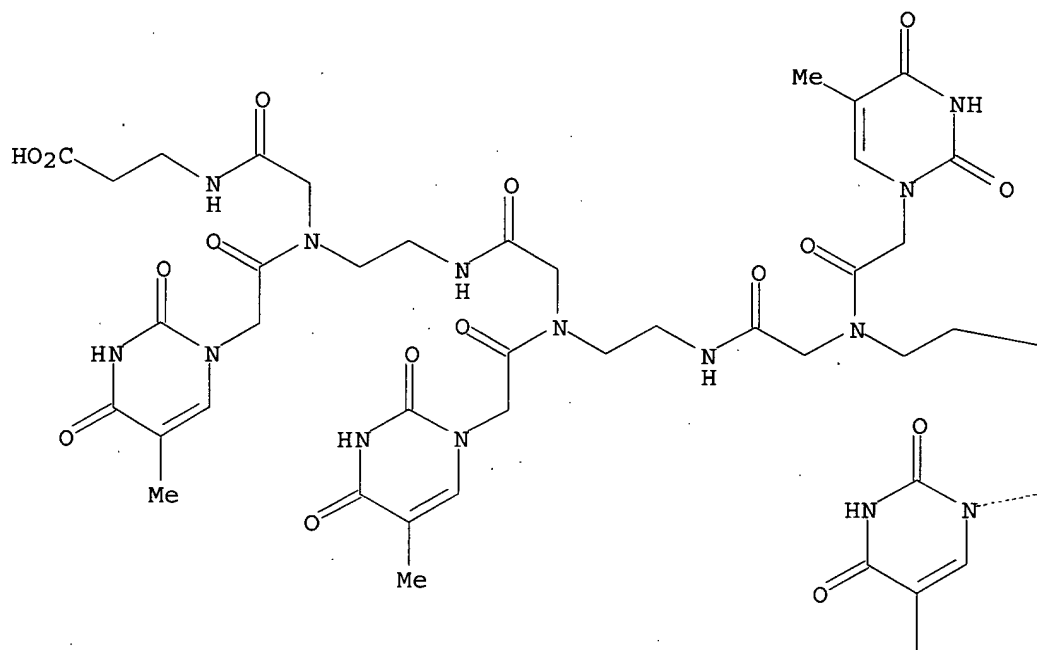


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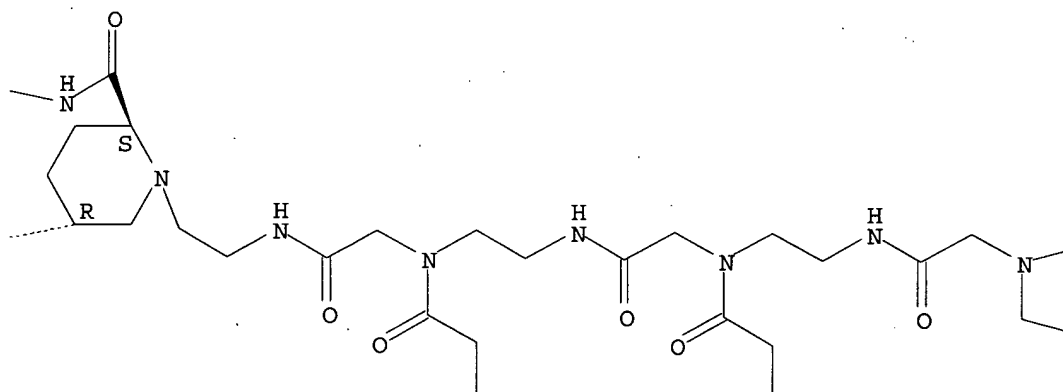
CN Peptide nucleic acid, (H-T-T-T-T-(2S,5R)-1-(2-aminoethyl)-5-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pip-T-T-T)-Bal-OH (9CI) (CA INDEX NAME)

Absolute stereochemistry.

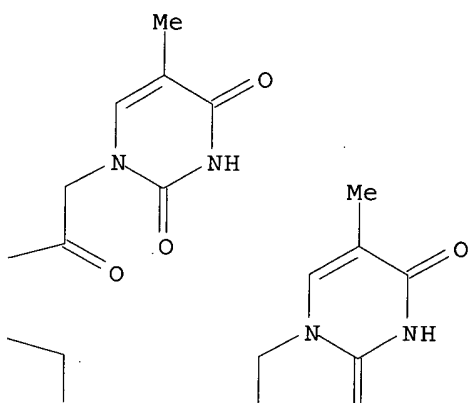
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PAGE 1-B



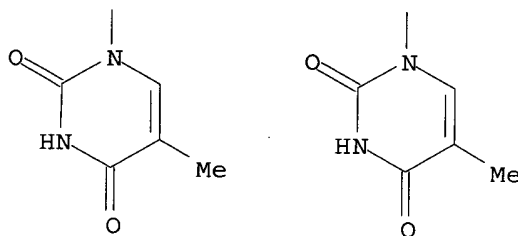
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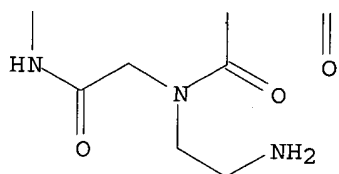
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PAGE 2-B



PAGE 2-C

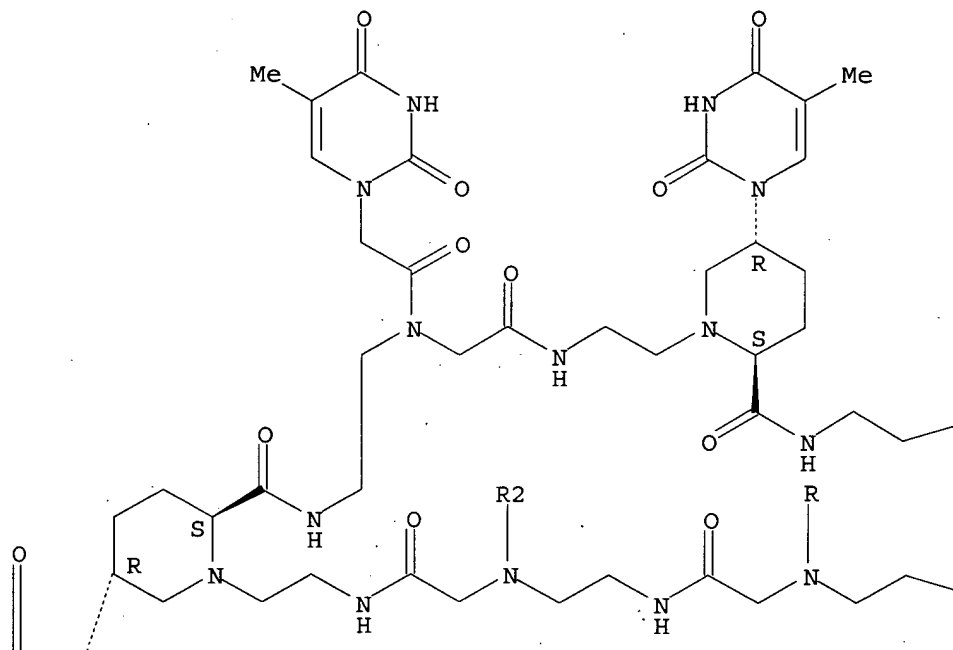


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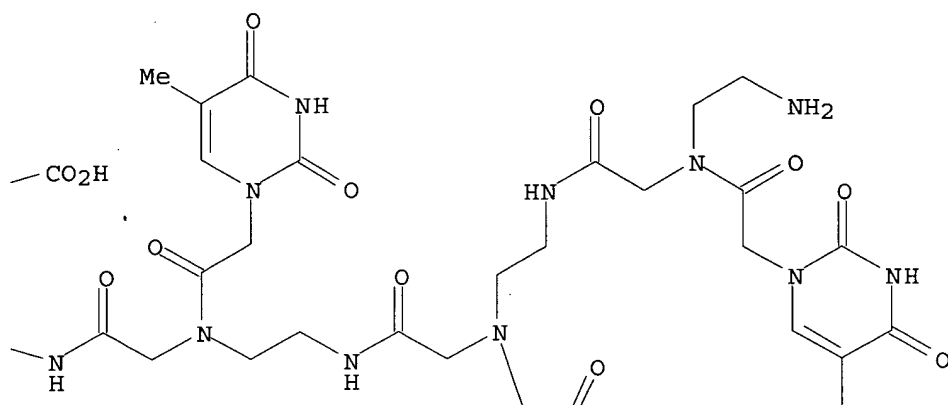
CN Peptide nucleic acid, (H-T-T-T-T-T-(2S,5R)-1-(2-aminoethyl)-5-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pip-T)-(2S,5R)-1-(2-aminoethyl)-5-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pip-Bal-OH (9CI) (CA INDEX NAME)

Absolute stereochemistry.

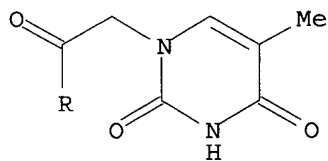
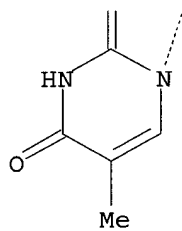
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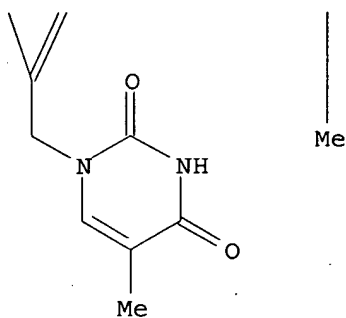
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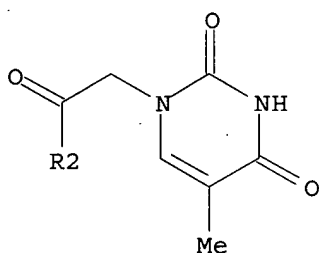
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PAGE 2-B



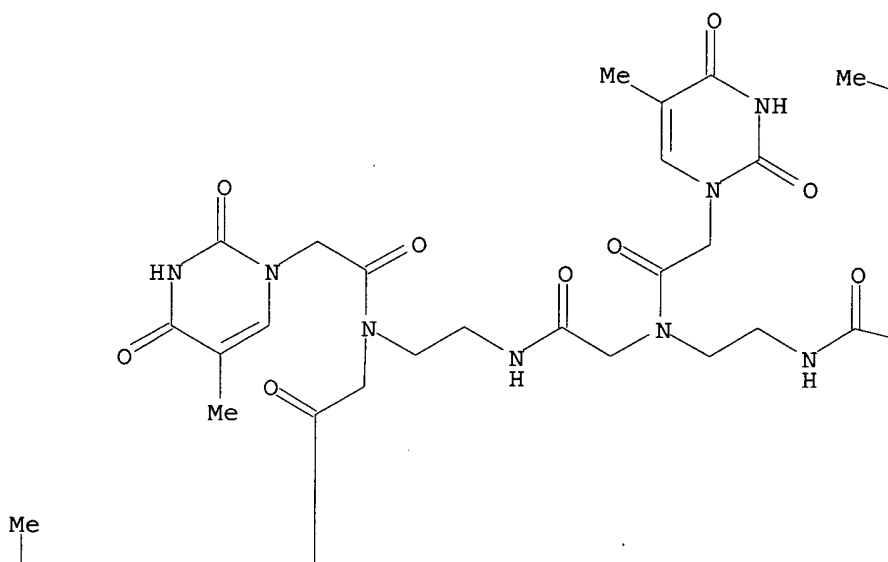
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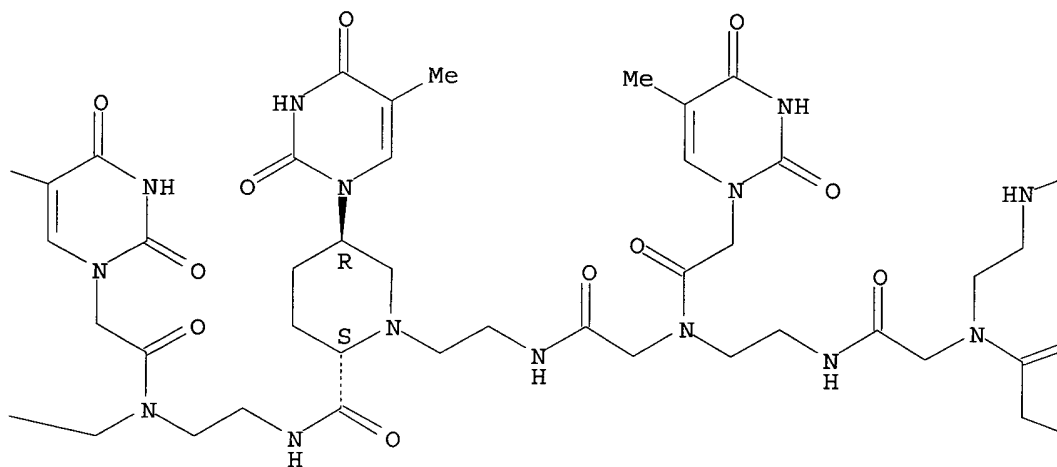
RN 695183-70-1 HCAPLUS
CN Peptide nucleic acid, (H-T-T-T-(2S,5R)-1-(2-aminoethyl)-5-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pip-T-T-T)-(2S,5R)-1-(2-aminoethyl)-5-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pip-Bal-OH (9CI) (CA INDEX NAME)

Absolute stereochemistry.

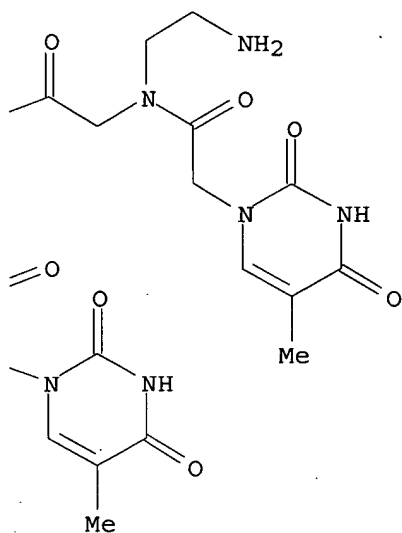
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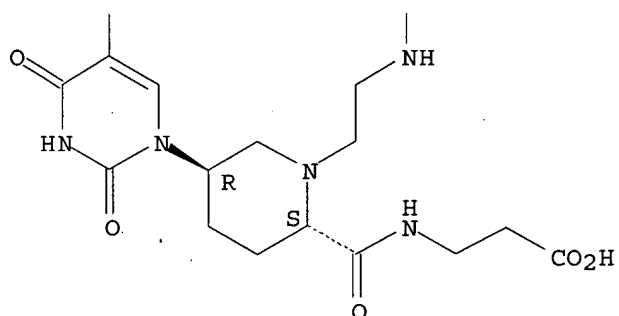
PAGE 1-B



PAGE 1-C



PAGE 2-A

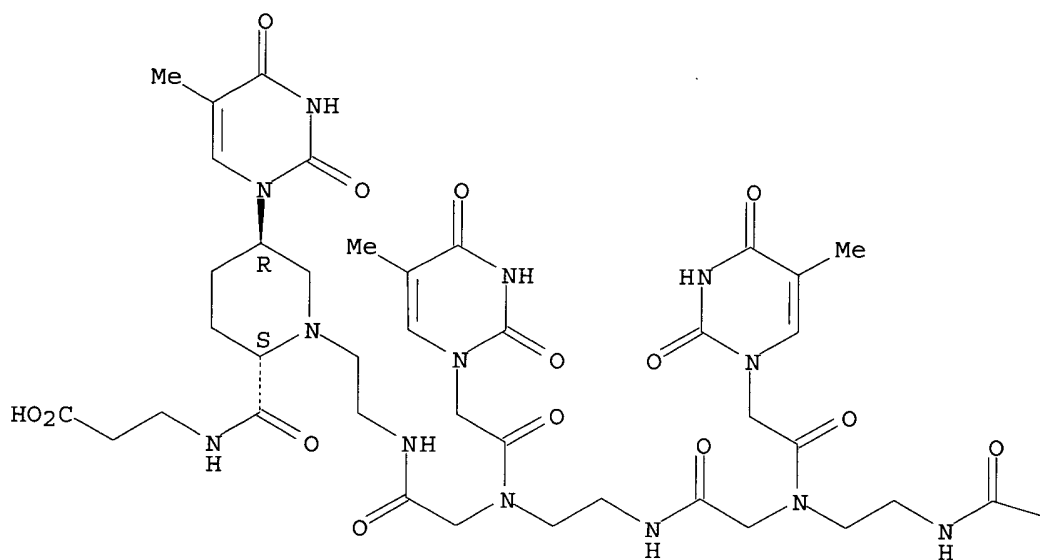


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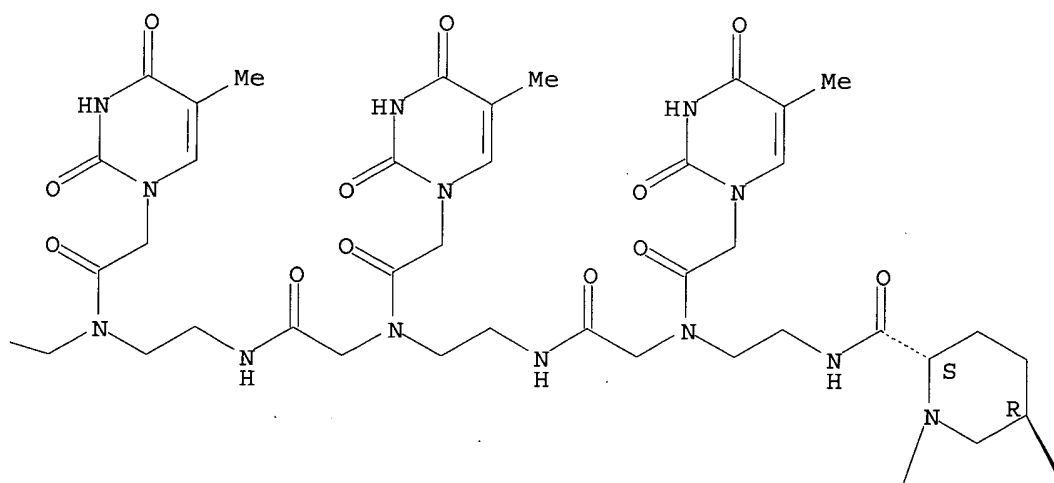
CN Peptide nucleic acid, (H-T-(2S,5R)-1-(2-aminoethyl)-5-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pip-T-T-T-T-T)-(2S,5R)-1-(2-aminoethyl)-5-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pip-Bal-OH (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



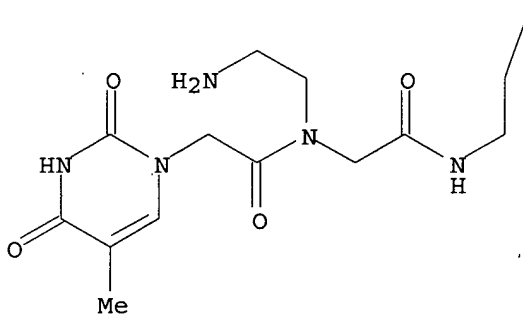
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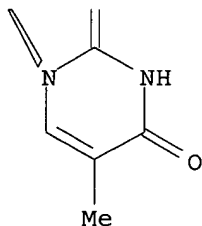
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PAGE 2-B



PAGE 2-C

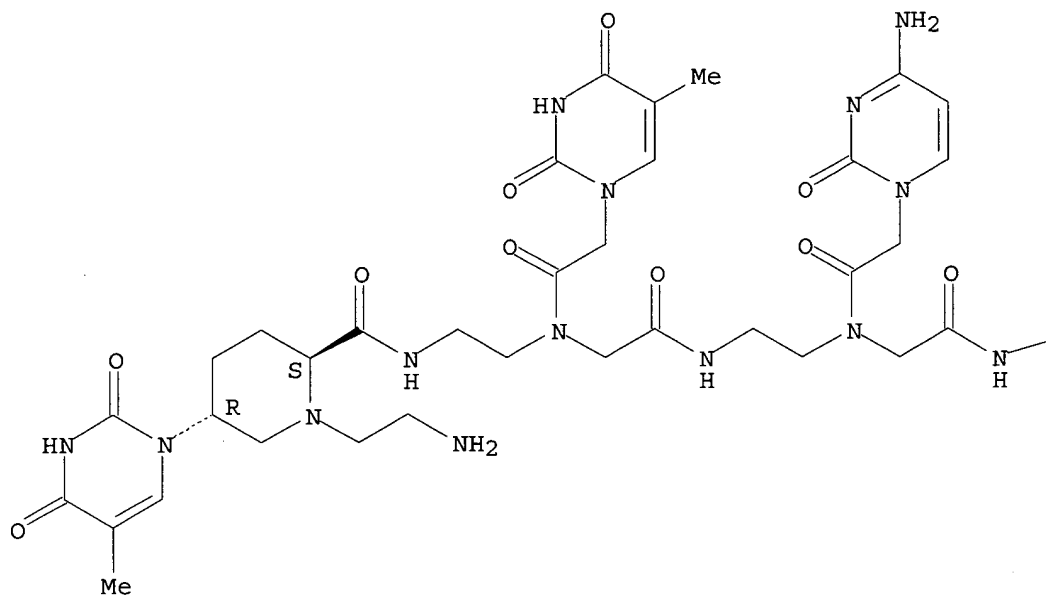


RN 695183-72-3 HCAPLUS
 CN Peptide nucleic acid, ([[(2S,5R)-1-(2-aminoethyl)-5-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-2-piperidinyl]carbonyl]-T-C-T-C-T-T-T)-Bal-OH

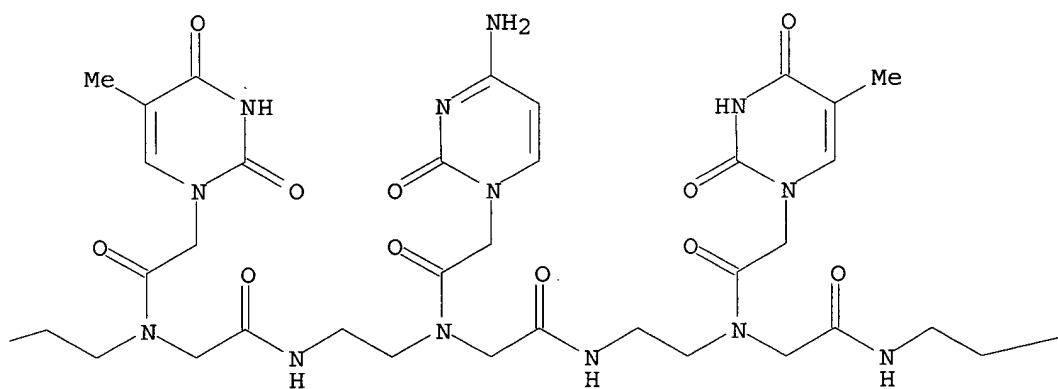
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

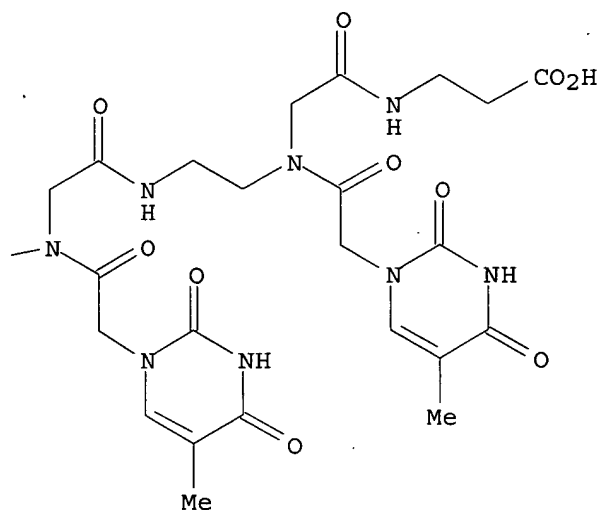
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PAGE 1-B

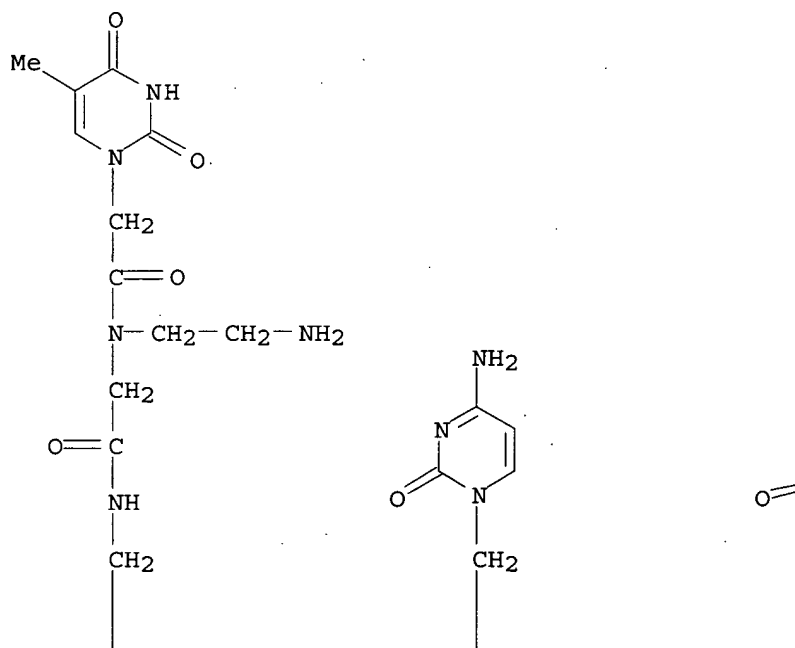


PAGE 1-C

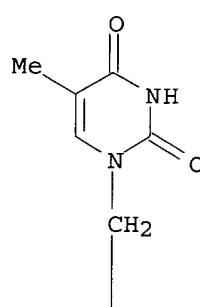
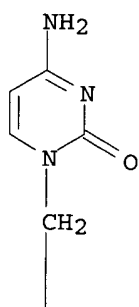
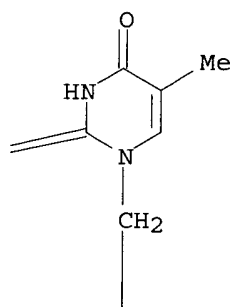


RN 695183-73-4 HCAPLUS
 CN Peptide nucleic acid, (H-T-T-C-T-C-T-T-T)-Bal-OH (9CI) (CA INDEX NAME)

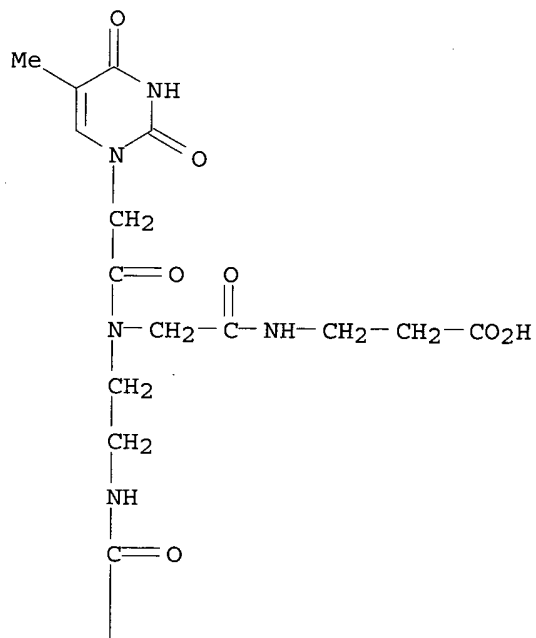
PAGE 1-A



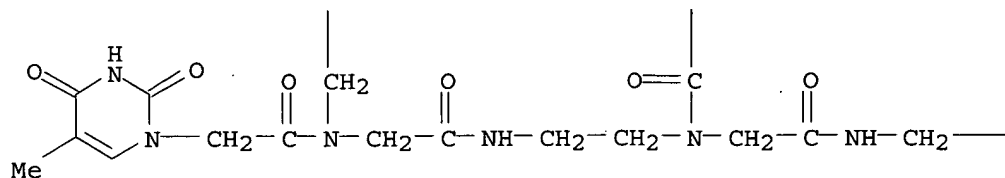
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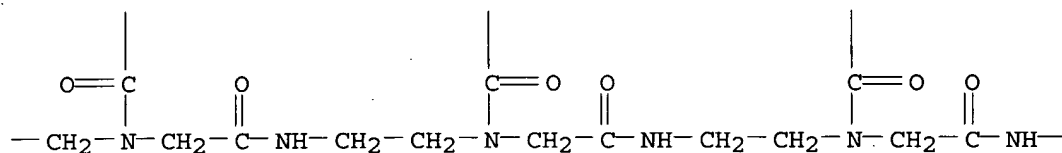
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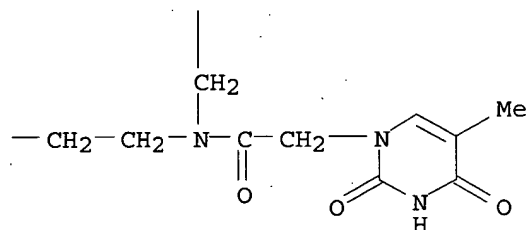
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PAGE 2-B



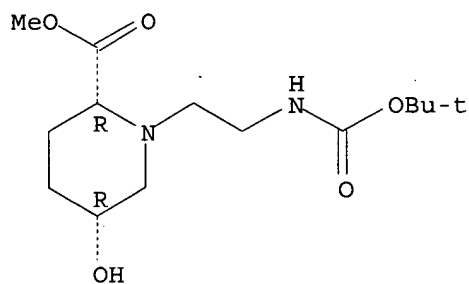
PAGE 2-C



RN 797801-63-9 HCAPLUS

CN 2-Piperidinecarboxylic acid, 1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl-5-hydroxy-, methyl ester, (2R,5R)-rel- (9CI) (CA INDEX NAME)

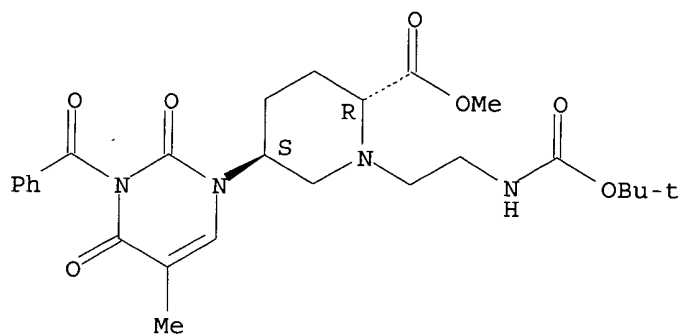
Relative stereochemistry.



RN 797801-64-0 HCAPLUS

CN 2-Piperidinecarboxylic acid, 5-(3-benzoyl-3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, methyl ester, (2R,5S)-rel- (9CI) (CA INDEX NAME)

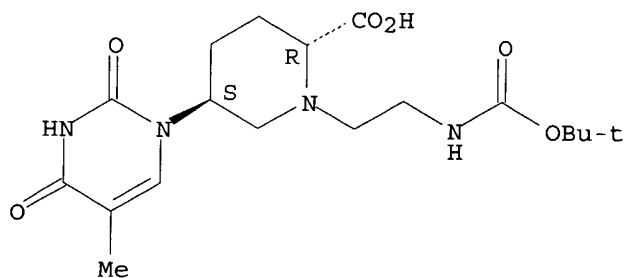
Relative stereochemistry.



RN 797801-65-1 HCAPLUS

CN 2-Piperidinecarboxylic acid, 5-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, (2R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

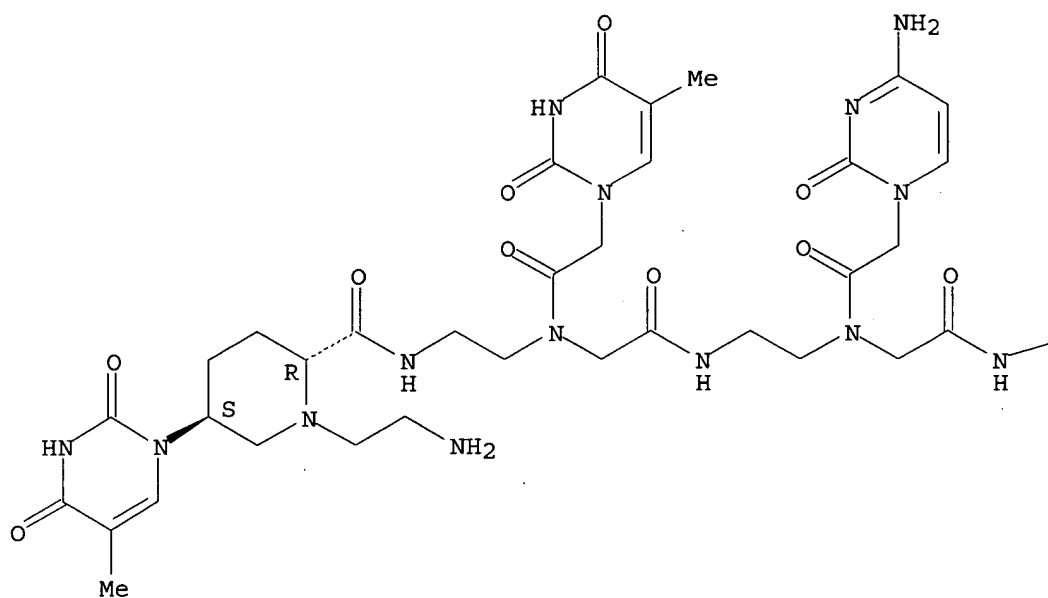


RN 797801-66-2 HCAPLUS

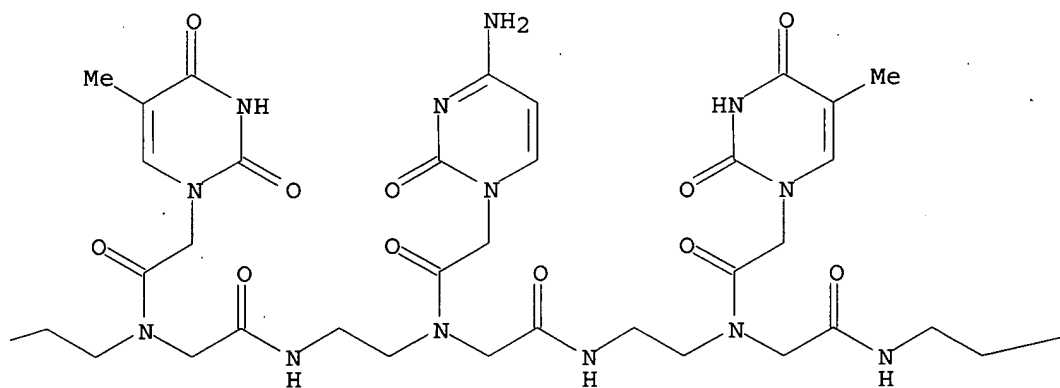
CN Peptide nucleic acid, ([[[(2R,5S)-1-(2-aminoethyl)-5-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-2-piperidinyl]carbonyl]-T-C-T-C-T-T-T)-Bal-OH (9CI) (CA INDEX NAME)

Absolute stereochemistry.

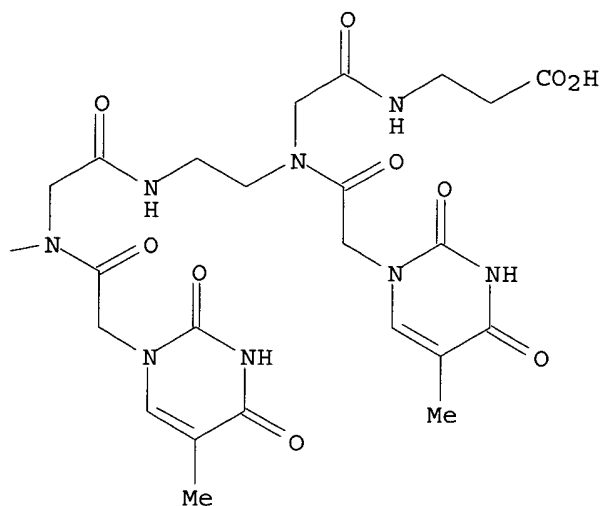
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PAGE 1-B



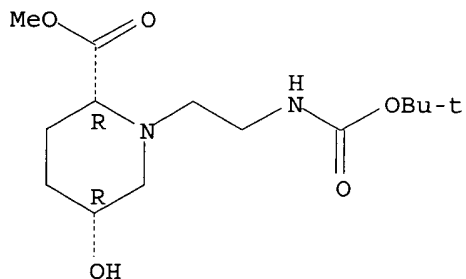
PAGE 1-C



RN 797801-69-5 HCAPLUS

CN 2-Piperidinecarboxylic acid, 1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-5-hydroxy-, methyl ester, (2R,5R)- (9CI) (CA INDEX NAME)

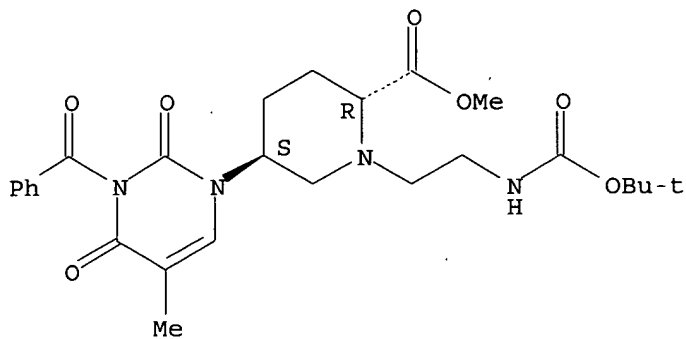
Absolute stereochemistry. Rotation (+).



RN 797801-70-8 HCAPLUS

CN 2-Piperidinecarboxylic acid, 5-(3-benzoyl-3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, methyl ester, (2R,5S)- (9CI) (CA INDEX NAME)

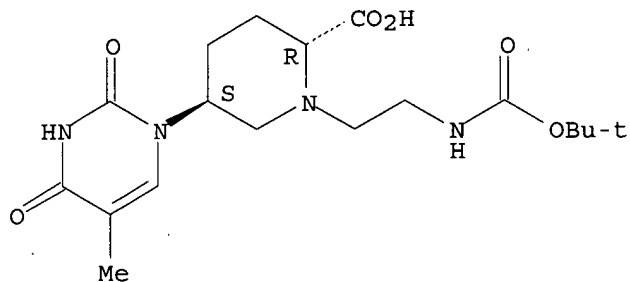
Absolute stereochemistry. Rotation (-).



RN 797801-71-9 HCAPLUS

CN 2-Piperidinecarboxylic acid, 5-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, (2R,5S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

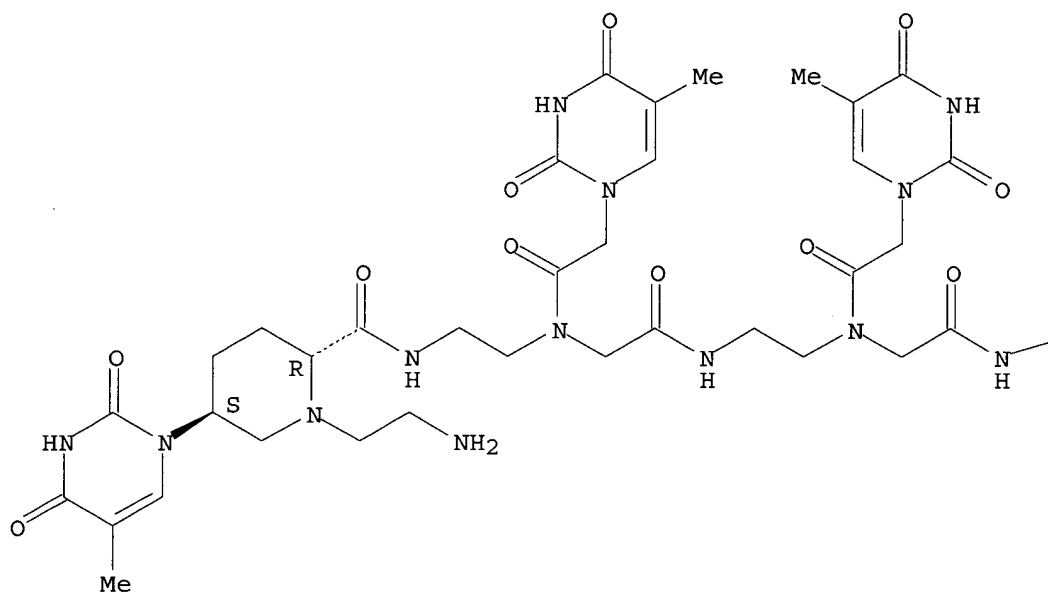


RN 797801-73-1 HCAPLUS

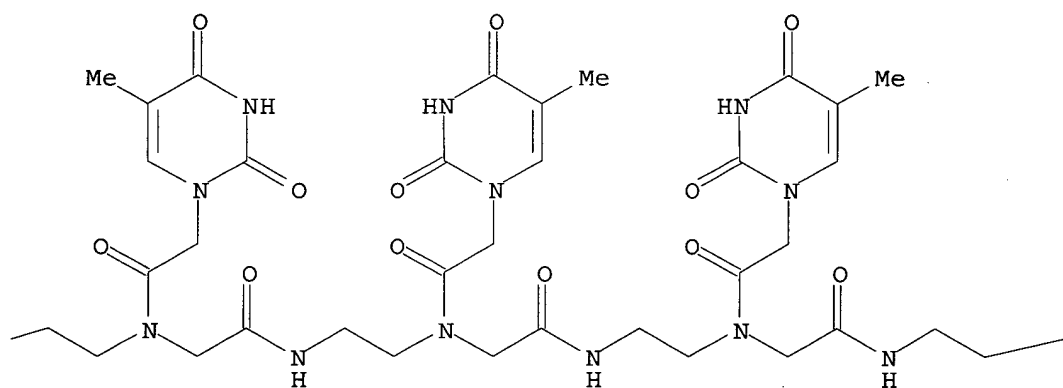
CN Peptide nucleic acid, ([[(2R,5S)-1-(2-aminoethyl)-5-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-2-piperidinyl]carbonyl]-T-T-T-T-T-T)-Bal-OH (9CI) (CA INDEX NAME)

Absolute stereochemistry.

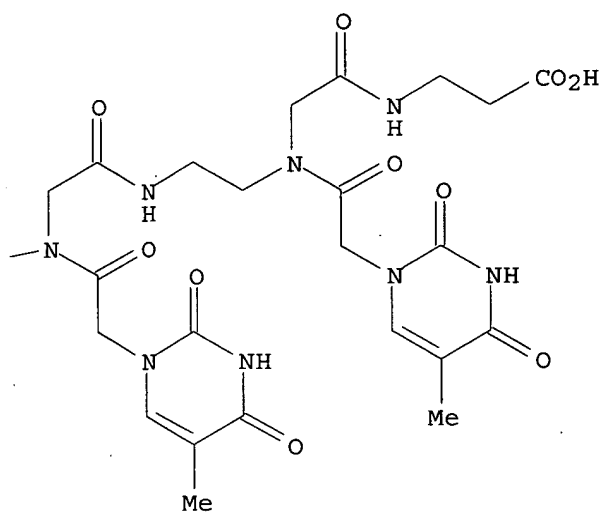
PAGE 1-A



PAGE 1-B



PAGE 1-C

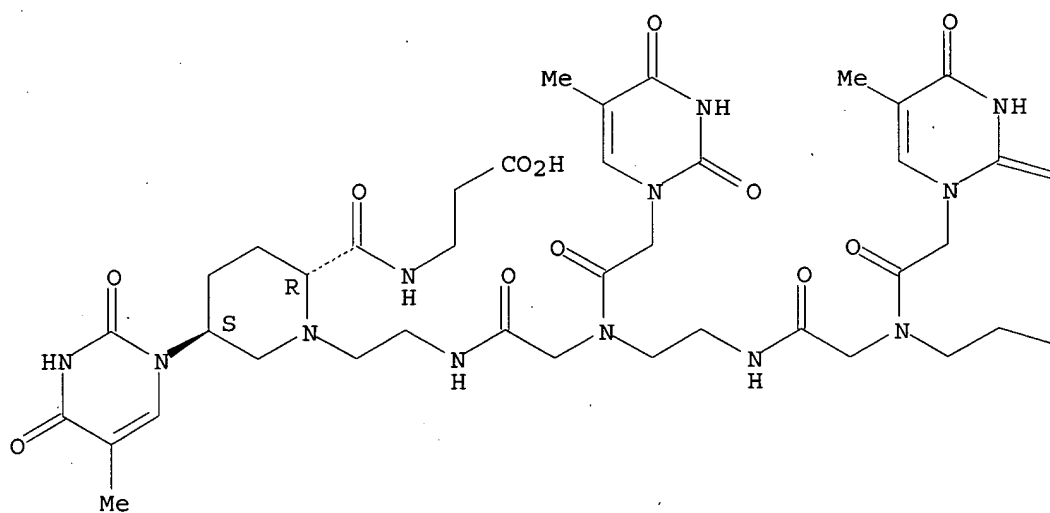


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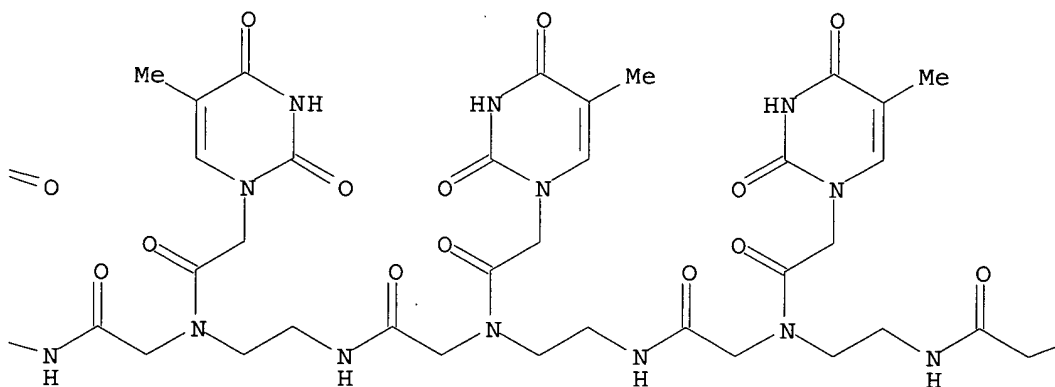
CN Peptide nucleic acid, (H-T-T-T-T-T-T-T)-(2R,5S)-1-(2-aminoethyl)-5-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pip-Bal-OH (9CI) (CA INDEX NAME)

Absolute stereochemistry.

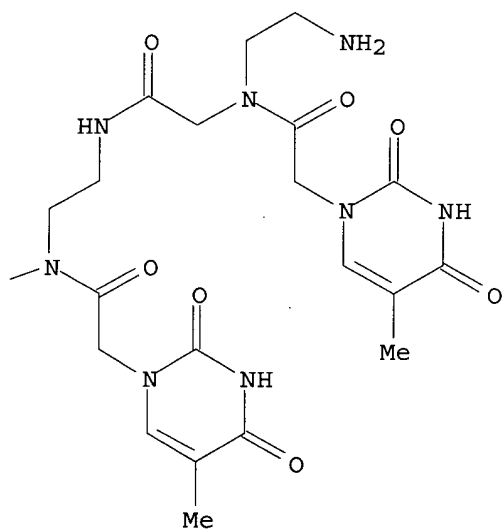
PAGE 1-A



PAGE 1-B



PAGE 1-C



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L38 ANSWER 2 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:245043 HCAPLUS

DOCUMENT NUMBER: 141:23882

TITLE: Chimeric peptide nucleic acids incorporating (2S,5R)-aminoethyl pipecolyl units: synthesis and DNA binding studies

AUTHOR(S): Shirude, Pravin S.; Kumar, Vaijayanti A.; Ganesh, Krishna N.

CORPORATE SOURCE: Division of Organic Chemistry (Synthesis), National Chemical Laboratory, Pune, 411008, India

SOURCE: Tetrahedron Letters (2004), 45(15), 3085-3088
CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:23882

AB Novel chiral six-membered PNA analog (2S,5R)-1-(N-Boc-aminoethyl)-5-(thymine-1-yl)pipecolic acid (Boc = tert-butoxycarbonyl), aeipPNA, was synthesized and incorporated into PNA sequences to effect stabilization of complexes with target complementary DNA. This is the first example where a six membered-PNA is shown to be capable of forming stable complexes with DNA and further expands the repertoire of cyclic PNA analogs.

CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 6, 33

IT 695183-80-3P 695183-82-5P 700382-81-6P 700382-82-7P
700382-83-8P 700382-84-9P 700382-85-0P 700382-86-1P 700382-87-2P
700382-88-3P 700382-89-4P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and DNA binding of chimeric peptide nucleic acids incorporating aminoethyl pipecolyl units)

IT 253307-86-7P 695183-56-3P 695183-59-6P
695183-62-1P 695183-64-3P 695183-65-4P
695183-68-7P 695183-69-8P 695183-70-1P
695183-71-2P 695183-72-3P 695183-73-4P

695183-75-6P 695183-78-9P 695596-03-3P 695596-04-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(preparation and DNA binding of chimeric peptide nucleic acids incorporating aminoethyl pipecolyl units)

IT 695183-80-3P 695183-82-5P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and DNA binding of chimeric peptide nucleic acids incorporating aminoethyl pipecolyl units)

RN 695183-80-3 HCAPLUS

CN Adenosine, 2'-deoxyadenylyl-(3'→5')-2'-deoxyadenylyl-(3'→5')-
2'-deoxyadenylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-
deoxyadenylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-
deoxyadenylyl-(3'→5')-2'-deoxy-, complex with peptide nucleic acid
([[(2S,5R)-1-(2-aminoethyl)-5-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-
pyrimidinyl)-2-piperidinyl]carbonyl]-T-C-T-C-T-T-T)-Bal-OH (1:2) (9CI)
(CA INDEX NAME)

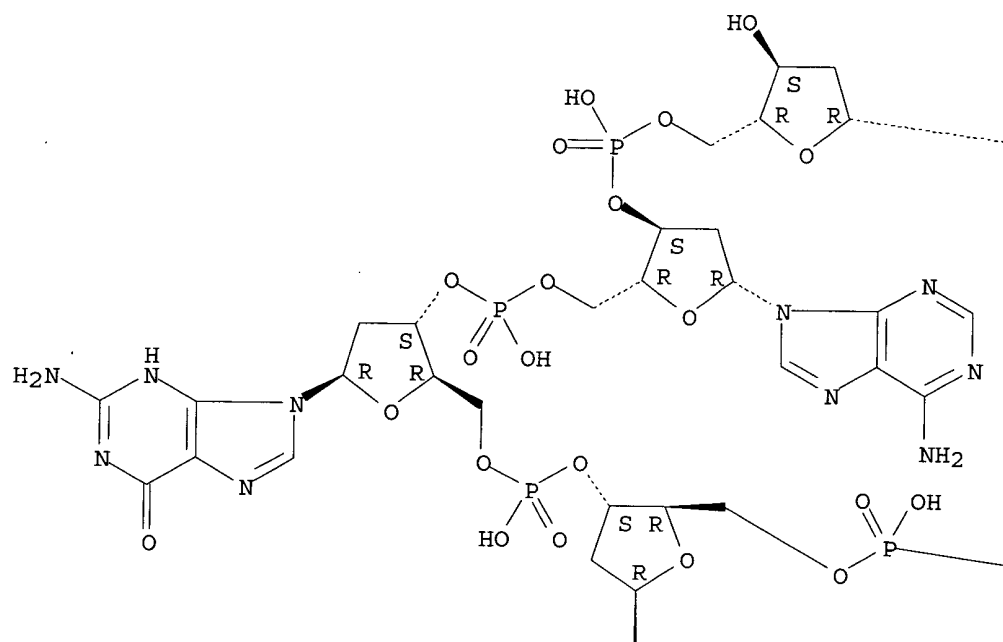
CM 1

CRN 695183-78-9

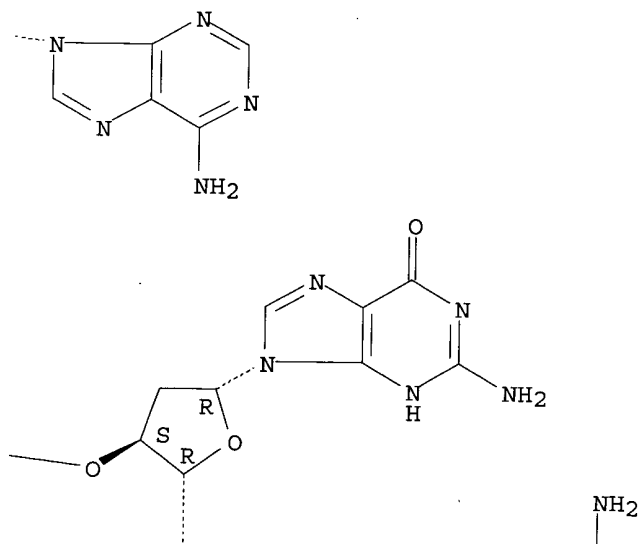
CMF C80 H97 N40 O40 P7

Absolute stereochemistry.

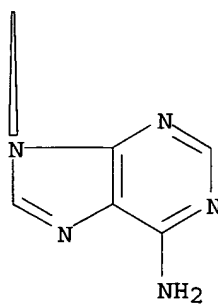
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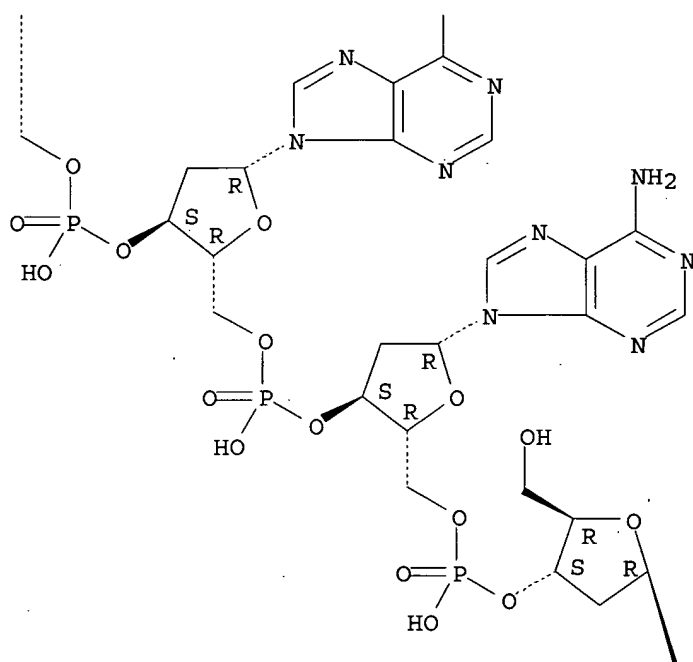
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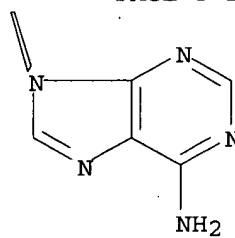
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PAGE 2-B



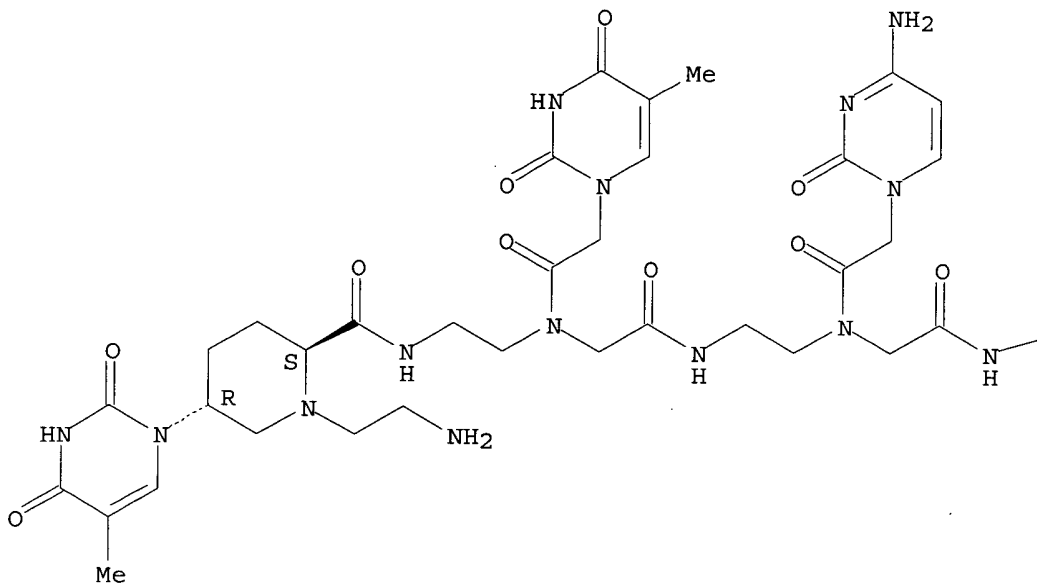
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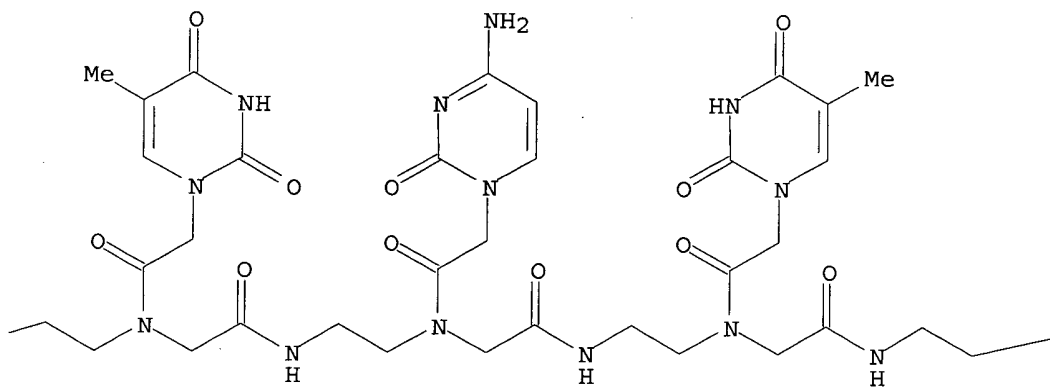
CRN 695183-72-3
CMF C91 H121 N35 O31

Absolute stereochemistry.

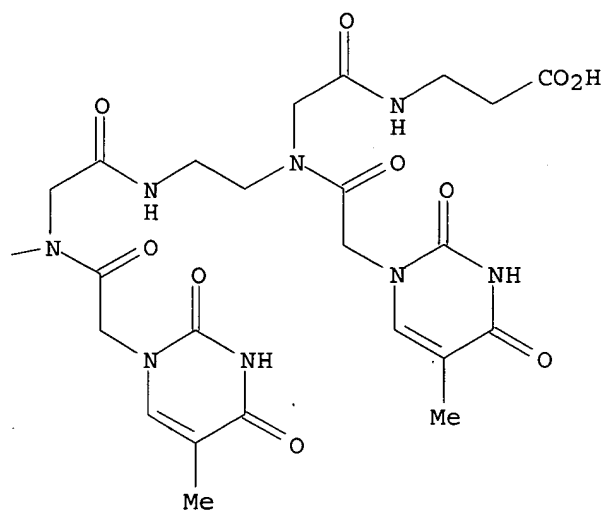
PAGE 1-A



PAGE 1-B



PAGE 1-C



RN 695183-82-5 HCAPLUS

CN Adenosine, 2'-deoxyadenylyl-(3'→5')-2'-deoxyadenylyl-(3'→5')-2'-deoxyadenylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxyadenylyl-(3'→5')-2'-deoxy-, complex with peptide nucleic acid (H-T-T-C-T-C-T-T-T)-Bal-OH (1:2) (9CI) (CA INDEX NAME)

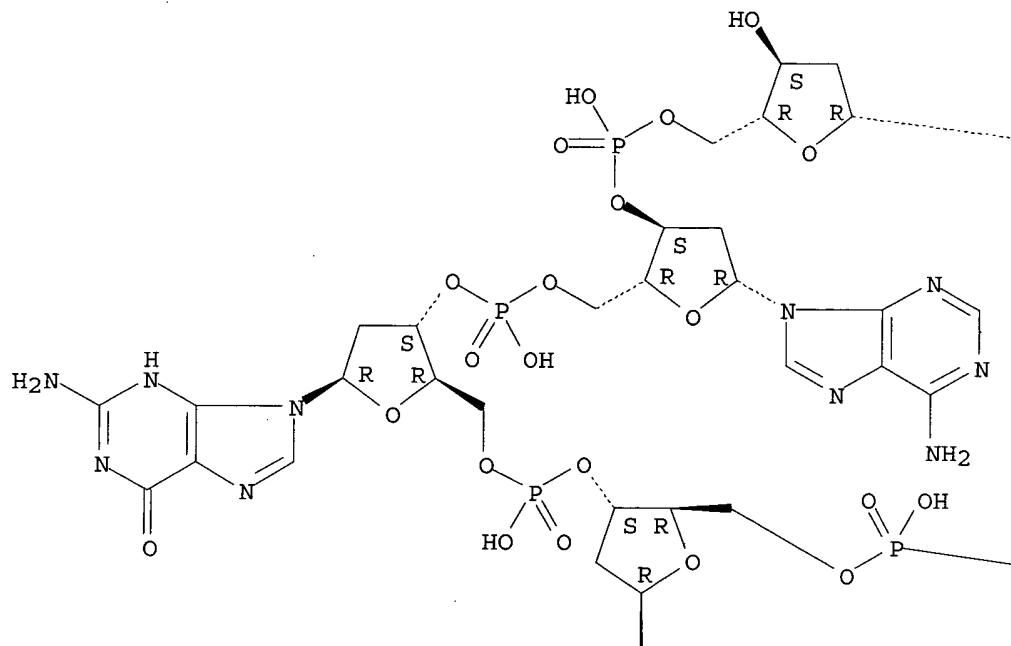
CM 1

CRN 695183-78-9

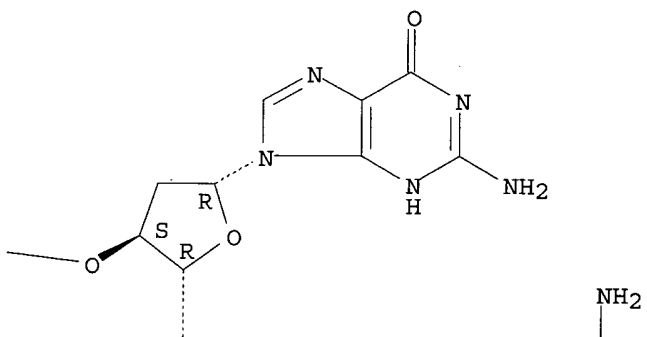
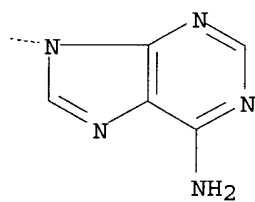
CMF C80 H97 N40 O40 P7

Absolute stereochemistry.

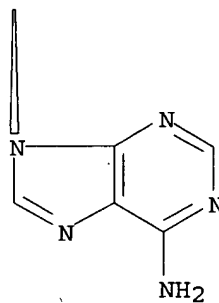
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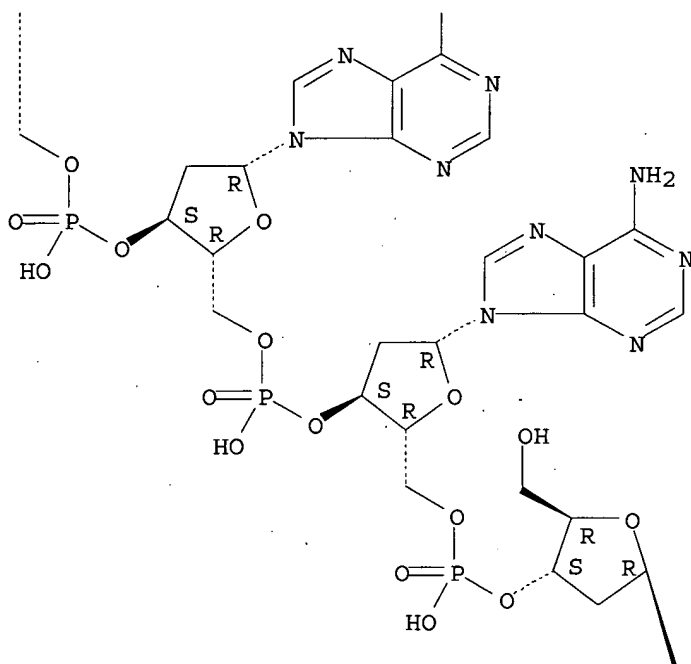
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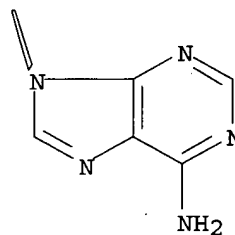
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PAGE 2-B

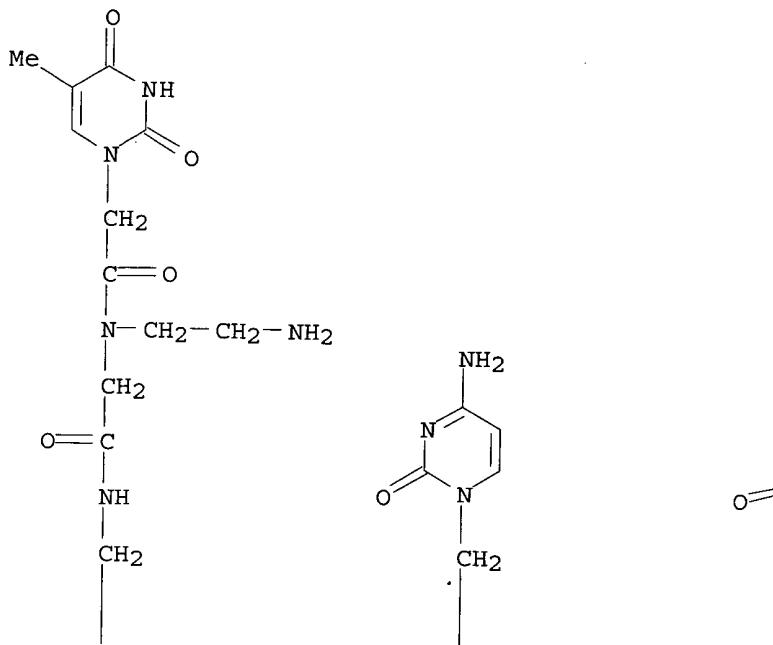


PAGE 3-B

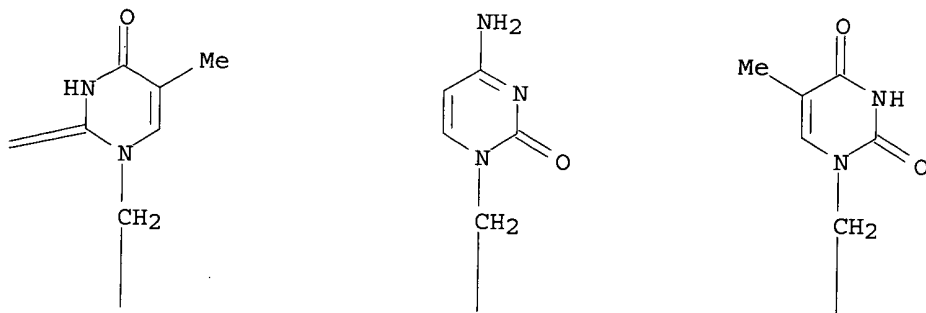


CRN 695183-73-4
CMF C89 H117 N35 O32

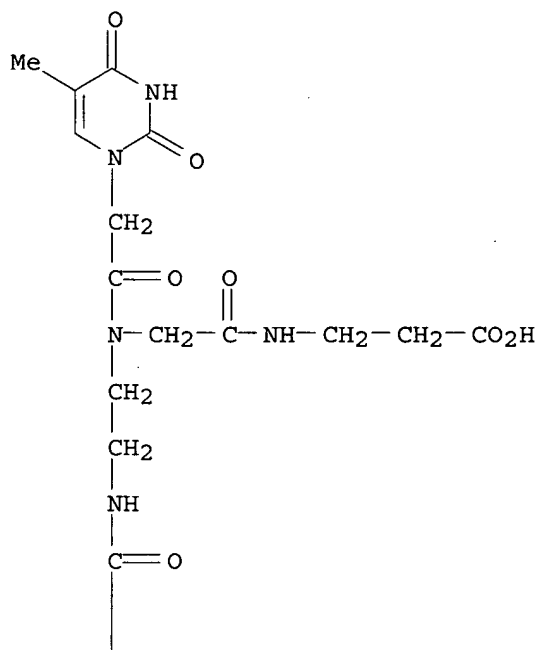
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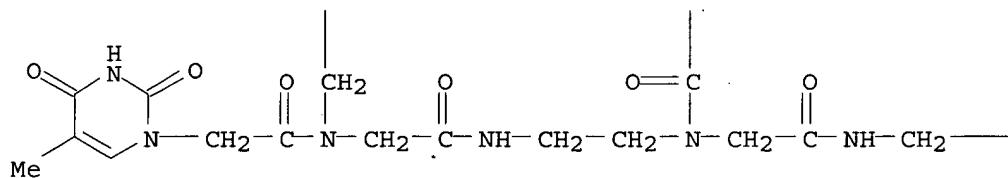
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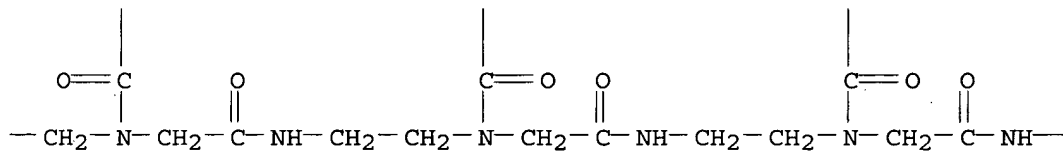
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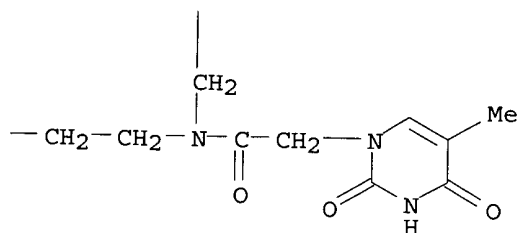
PAGE 2-A



PAGE 2-B



PAGE 2-C



IT 253307-86-7P 695183-56-3P 695183-59-6P
 695183-62-1P 695183-64-3P 695183-65-4P
 695183-68-7P 695183-69-8P 695183-70-1P
 695183-71-2P 695183-72-3P 695183-73-4P

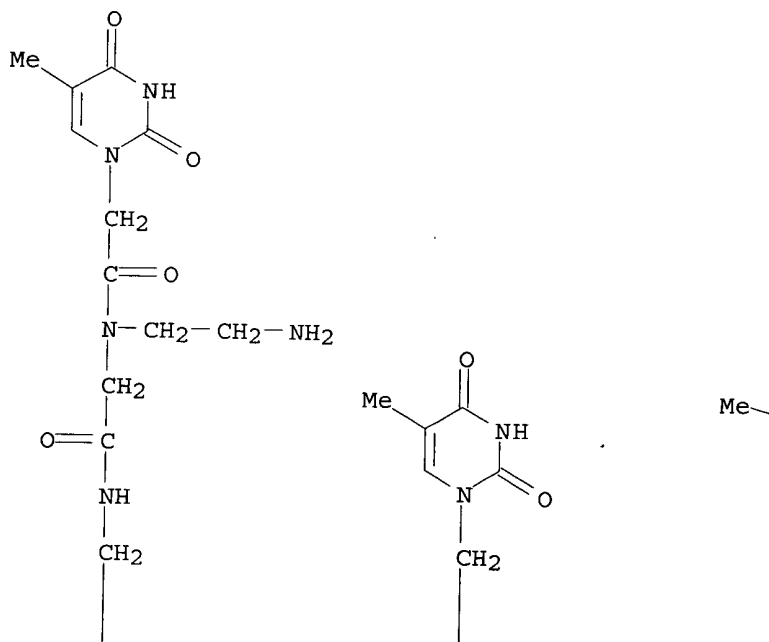
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 (Reactant or reagent)

(preparation and DNA binding of chimeric peptide nucleic acids incorporating
 aminoethyl pipecolyl units)

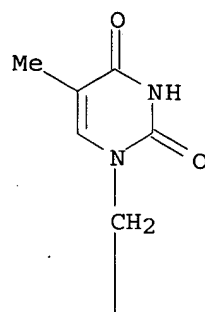
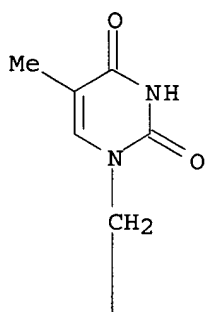
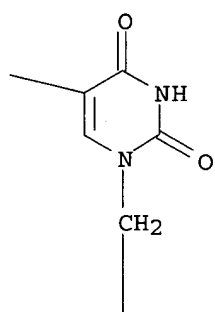
RN 253307-86-7 HCAPLUS

CN Peptide nucleic acid, (H-T-T-T-T-T-T-T)- β -ala-OH (9CI) (CA INDEX
 NAME)

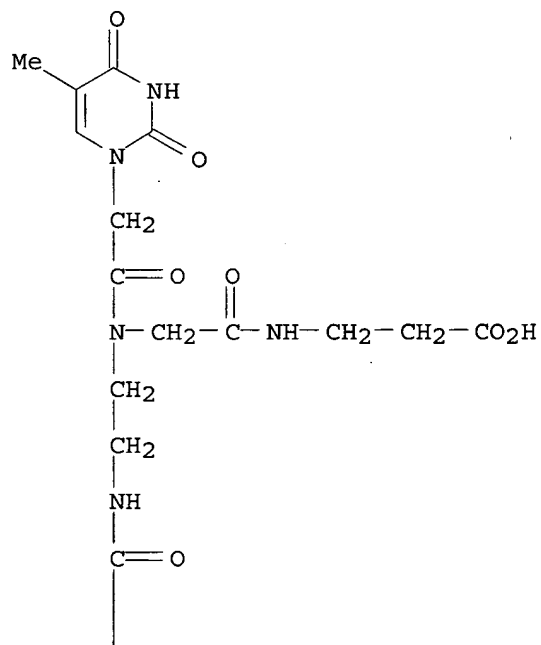
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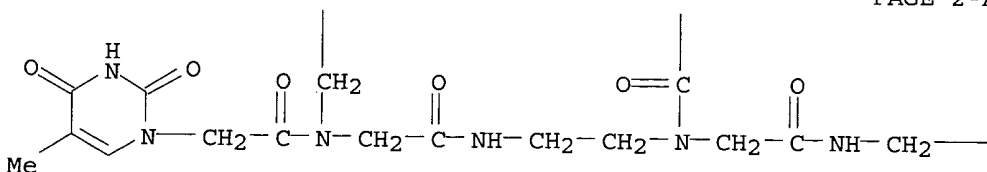
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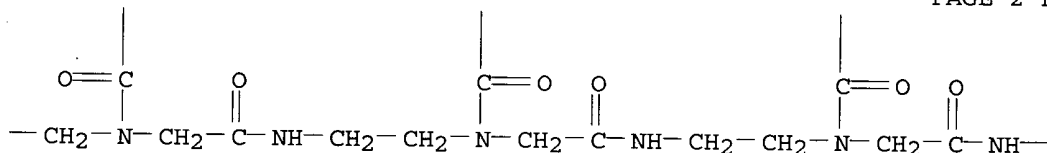
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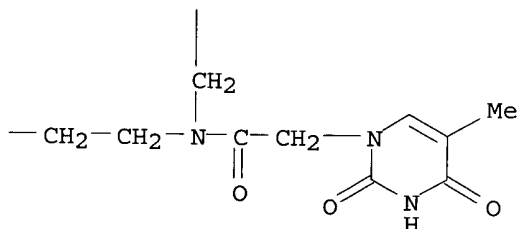
PAGE 2-A



PAGE 2-B



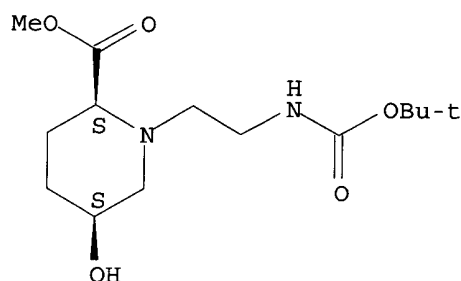
PAGE 2-C



RN 695183-56-3 HCAPLUS

CN 2-Piperidinecarboxylic acid, 1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-5-hydroxy-, methyl ester, (2S,5S)- (9CI) (CA INDEX NAME)

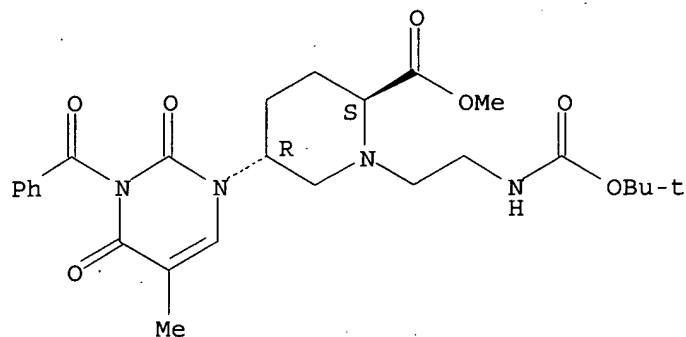
Absolute stereochemistry. Rotation (-).



RN 695183-59-6 HCAPLUS

CN 2-Piperidinecarboxylic acid, 5-(3-benzoyl-3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, methyl ester, (2S,5R)- (9CI) (CA INDEX NAME)

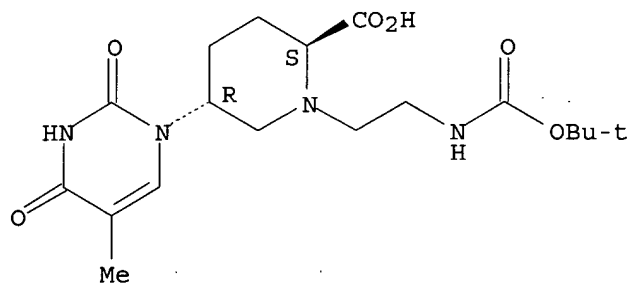
Absolute stereochemistry. Rotation (+).



RN 695183-62-1 HCAPLUS

CN 2-Piperidinecarboxylic acid, 5-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, (2S,5R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

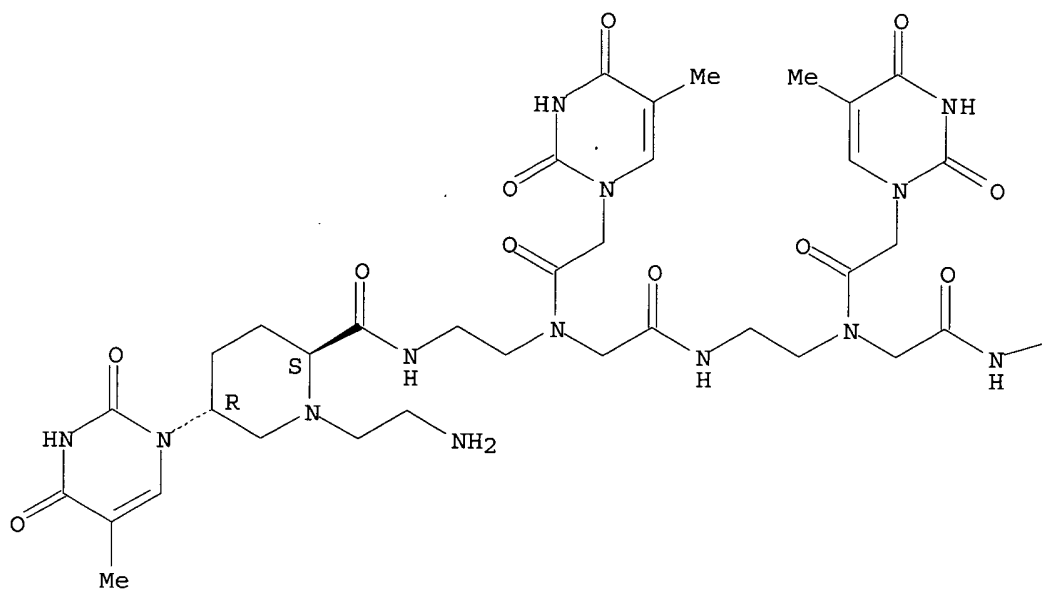


RN 695183-64-3 HCAPLUS

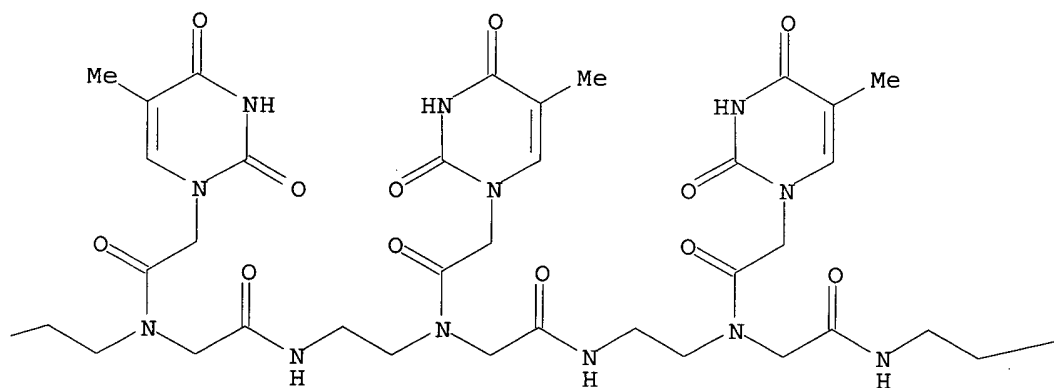
CN Peptide nucleic acid, ([[(2S,5R)-1-(2-aminoethyl)-5-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-2-piperidinyl]carbonyl]-T-T-T-T-T-T-T)-Bal-OH (9CI) (CA INDEX NAME)

Absolute stereochemistry.

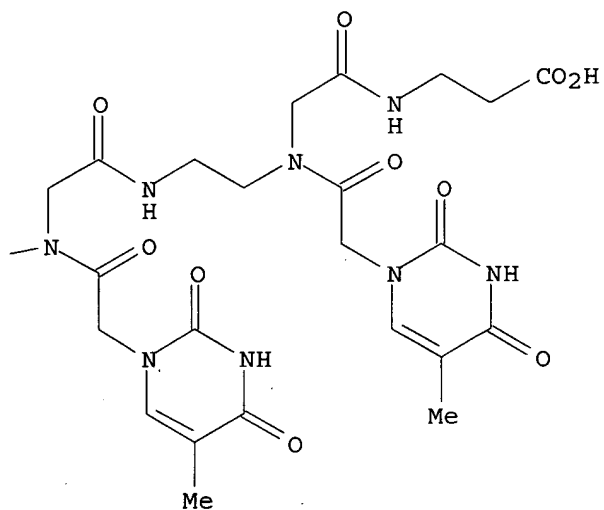
PAGE 1-A



PAGE 1-B



PAGE 1-C

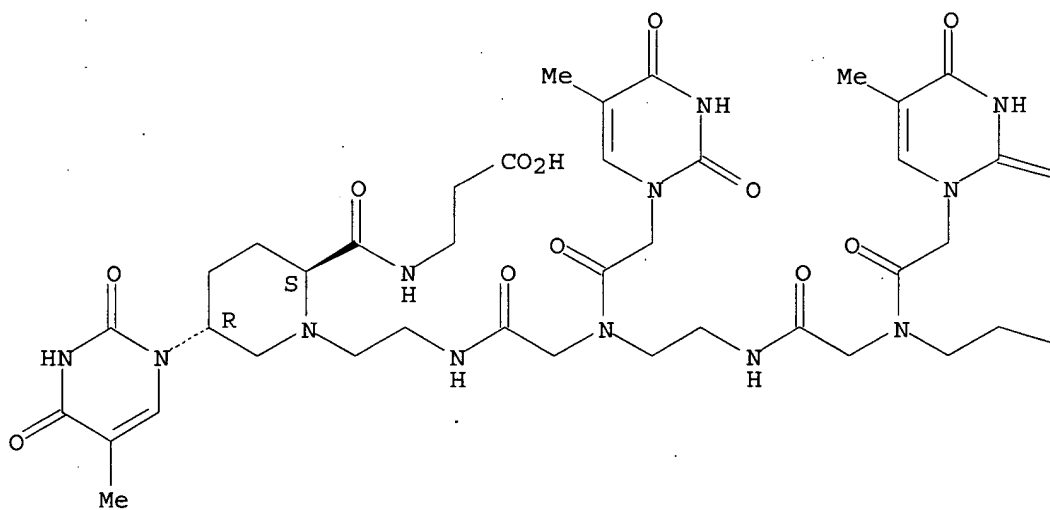


RN 695183-65-4 HCAPLUS

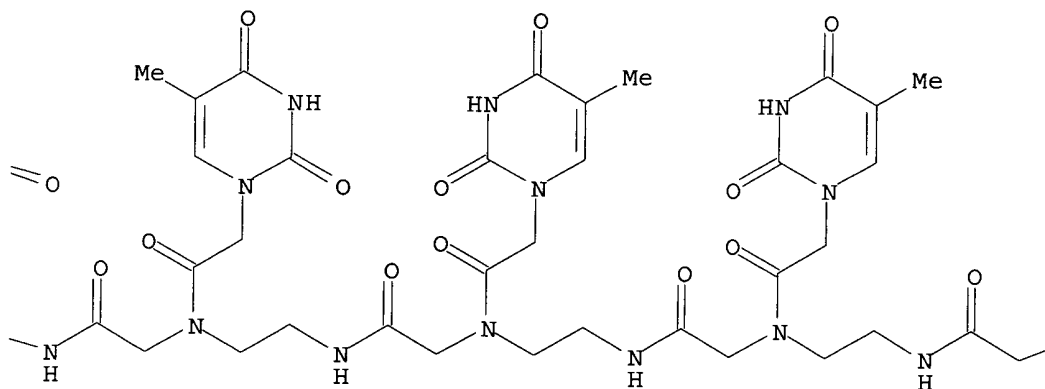
CN Peptide nucleic acid, (H-T-T-T-T-T-T-T)-(2S,5R)-1-(2-aminoethyl)-5-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pip-Bal-OH (9CI) (CA INDEX NAME)

Absolute stereochemistry.

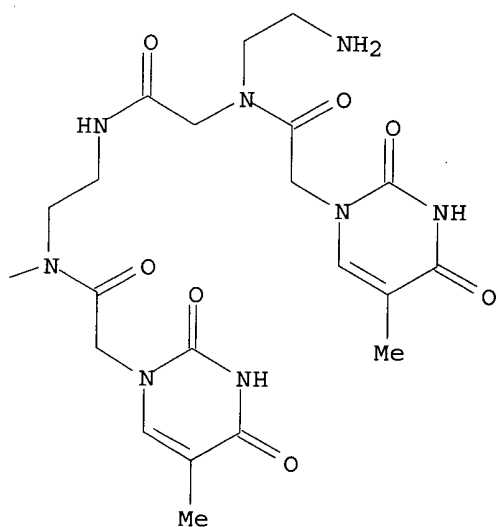
PAGE 1-A



PAGE 1-B



PAGE 1-C

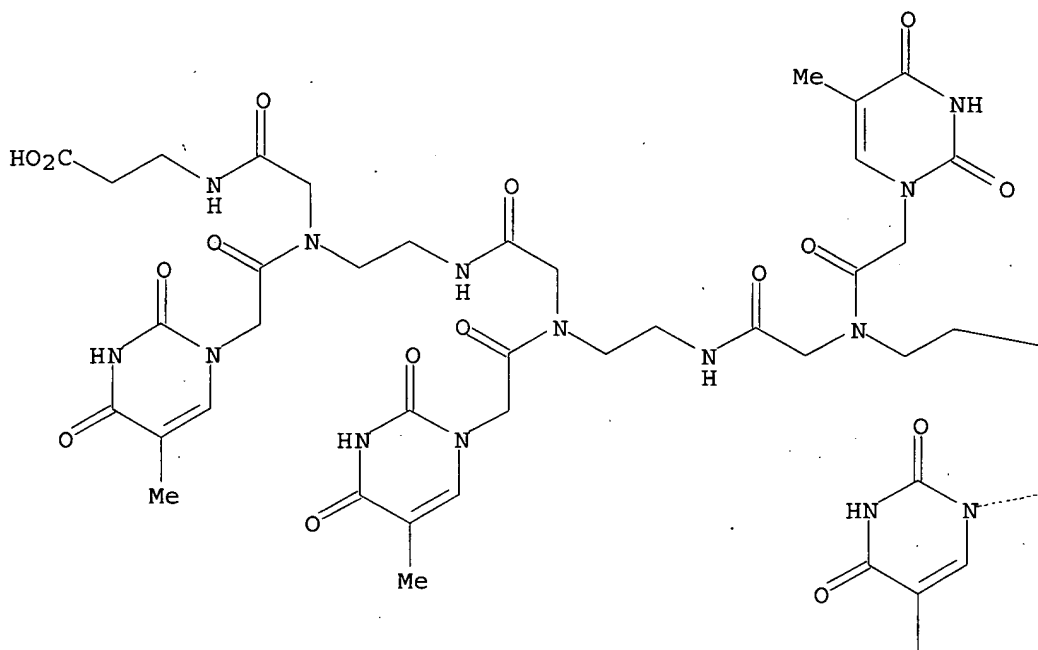


RN 695183-68-7 HCAPLUS

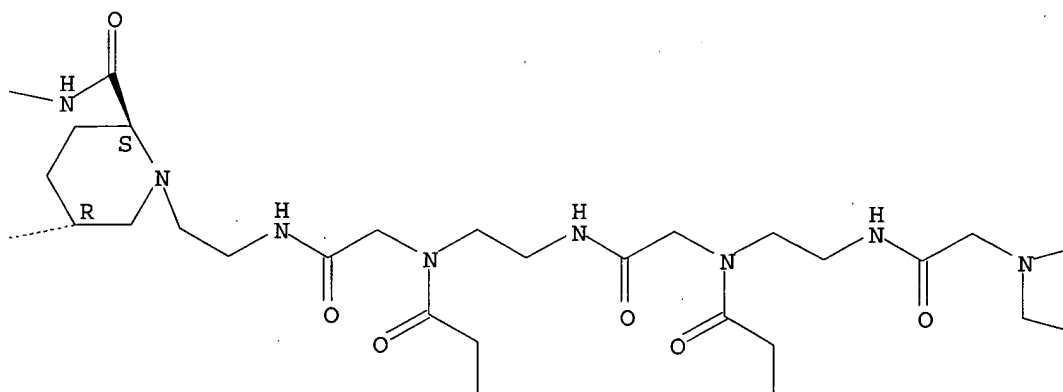
CN Peptide nucleic acid, (H-T-T-T-T-(2S,5R)-1-(2-aminoethyl)-5-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pip-T-T-T)-Bal-OH (9CI) (CA INDEX NAME)

Absolute stereochemistry.

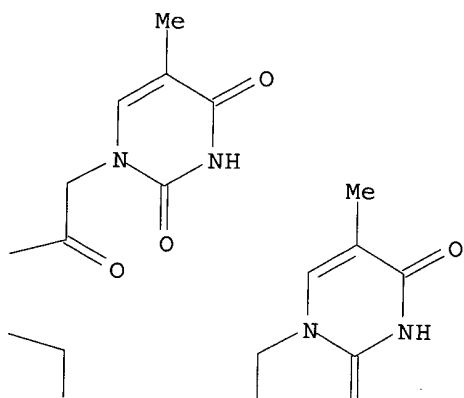
PAGE 1-A



PAGE 1-B



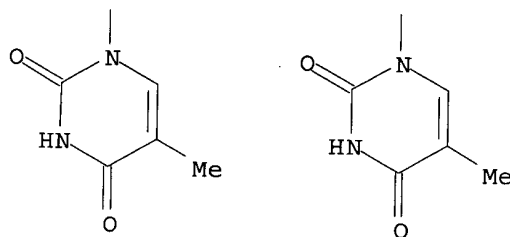
PAGE 1-C



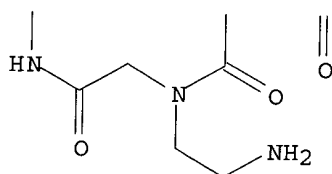
PAGE 2-A



PAGE 2-B



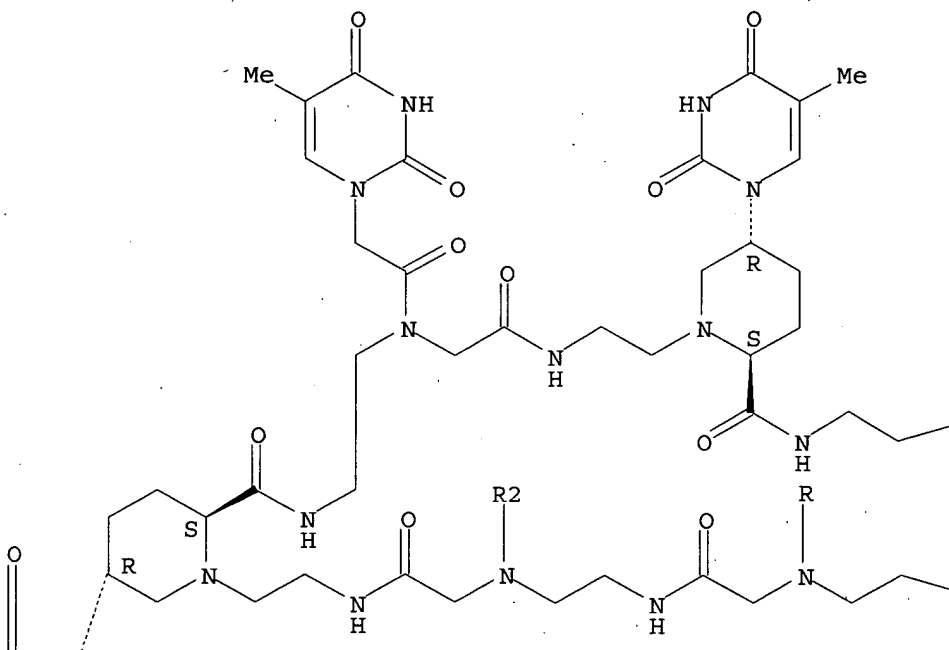
PAGE 2-C



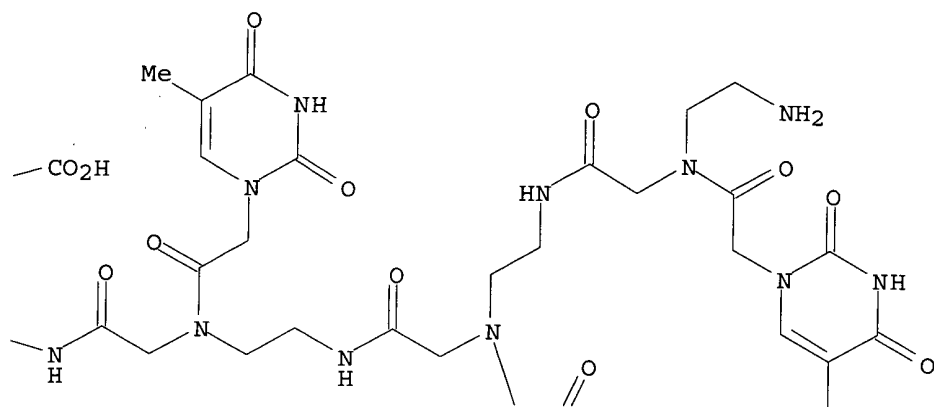
RN 695183-69-8 HCAPLUS
CN Peptide nucleic acid, (H-T-T-T-T-T-(2S,5R)-1-(2-aminoethyl)-5-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pip-T)-(2S,5R)-1-(2-aminoethyl)-5-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pip-Bal-OH (9CI) (CA INDEX NAME)

Absolute stereochemistry.

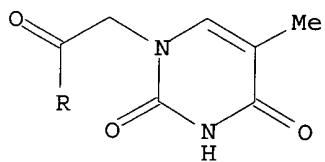
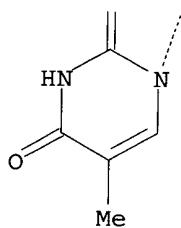
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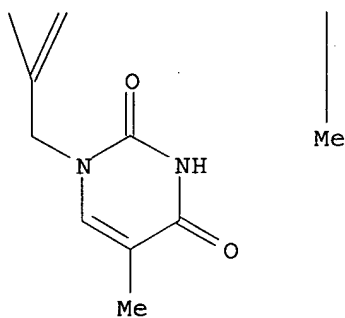
PAGE 1-B



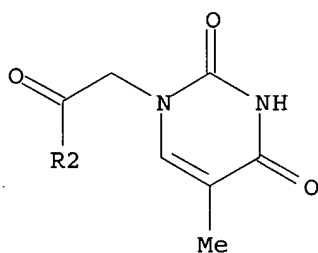
PAGE 2-A



PAGE 2-B



PAGE 3-A

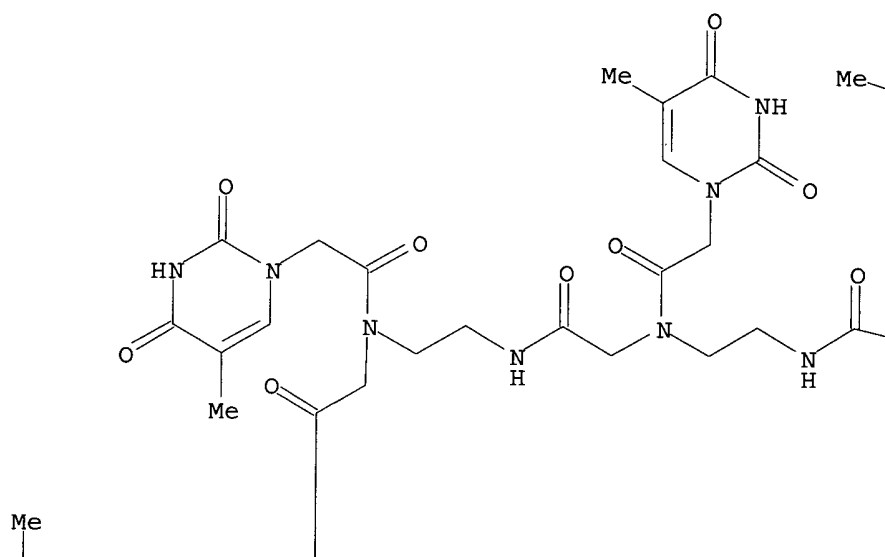


RN 695183-70-1 HCAPLUS

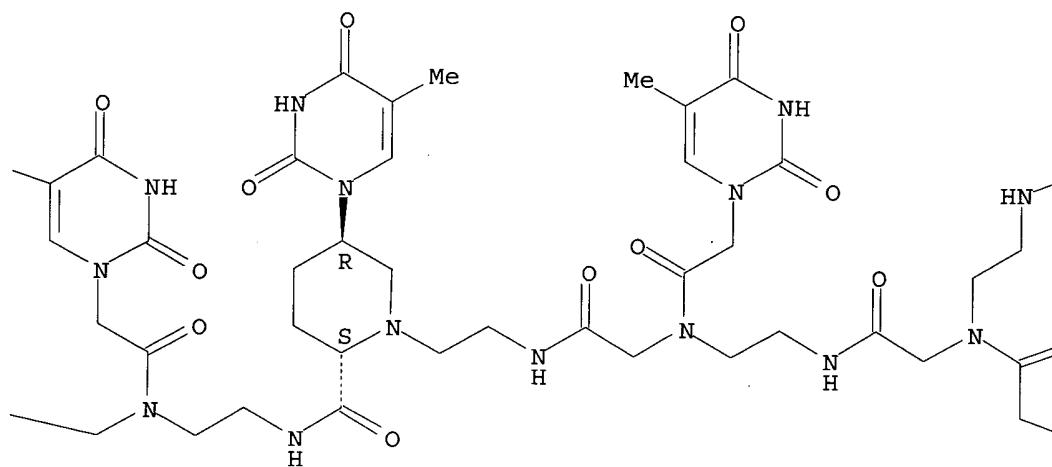
CN Peptide nucleic acid, (H-T-T-T-(2S,5R)-1-(2-aminoethyl)-5-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pip-T-T-T)-(2S,5R)-1-(2-aminoethyl)-5-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pip-Bal-OH (9CI) (CA INDEX NAME)

Absolute stereochemistry.

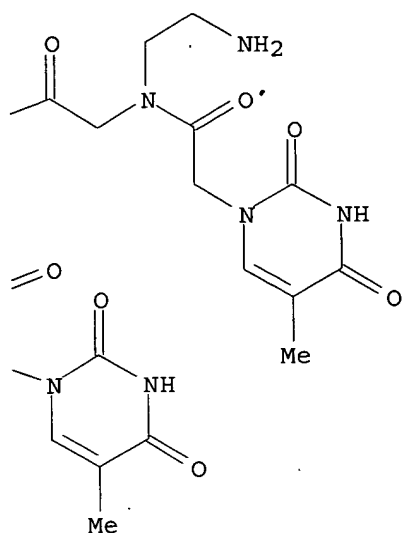
PAGE 1-A



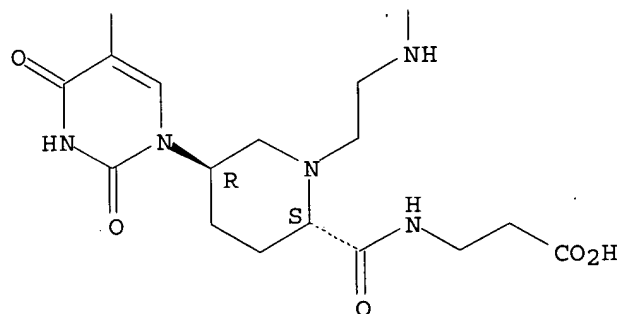
PAGE 1-B



PAGE 1-C



PAGE 2-A



RN 695183-71-2 HCAPLUS

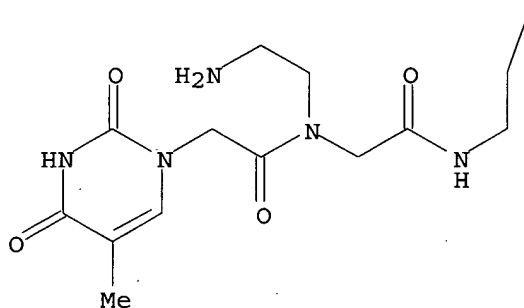
CN Peptide nucleic acid, (H-T-(2S,5R)-1-(2-aminoethyl)-5-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pip-T-T-T-T-T)-(2S,5R)-1-(2-aminoethyl)-5-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pip-Bal-OH (9CI) (CA INDEX NAME)

Absolute stereochemistry.

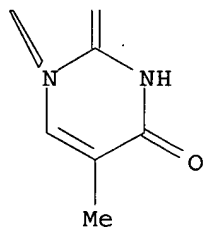
PAGE 1-C



PAGE 2-B



PAGE 2-C

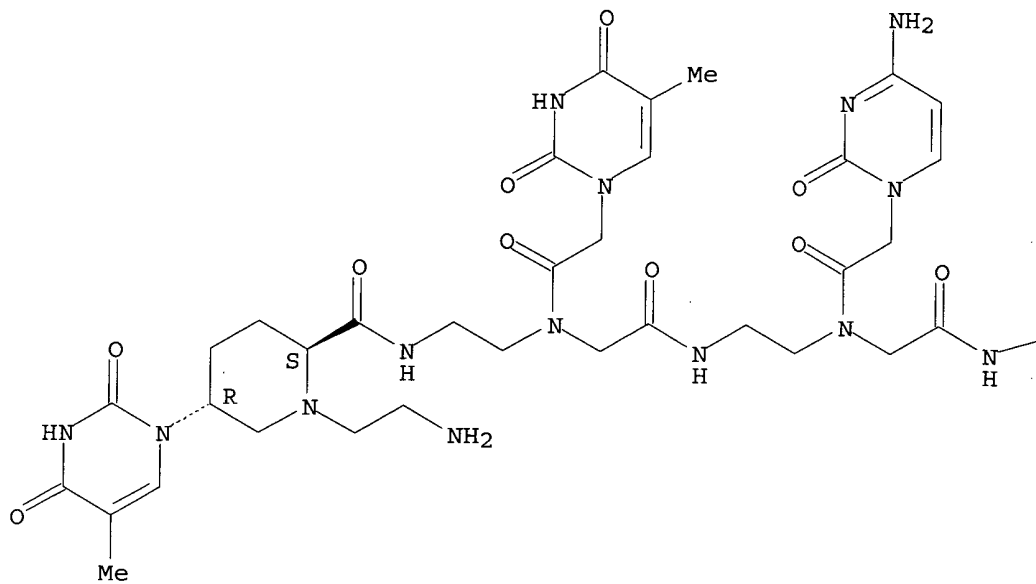


RN 695183-72-3 HCAPLUS
 CN Peptide nucleic acid, ([[(2S,5R)-1-(2-aminoethyl)-5-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-2-piperidinyl]carbonyl]-T-C-T-C-T-T-T)-Bal-OH

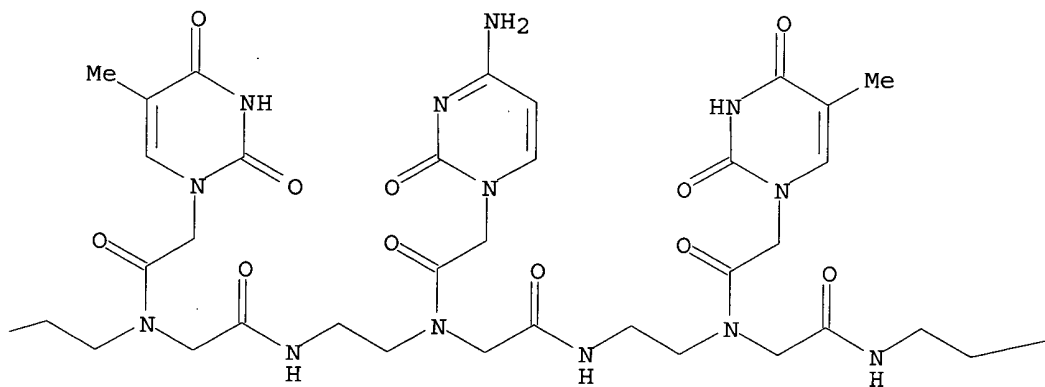
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

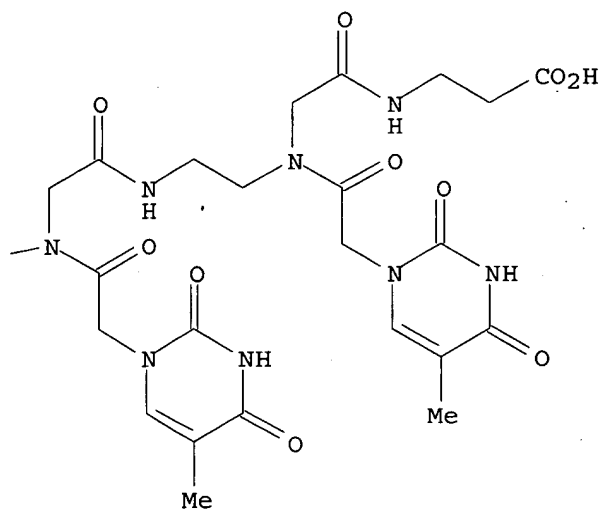
PAGE 1-A



PAGE 1-B



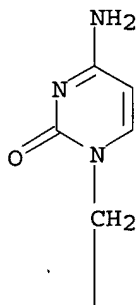
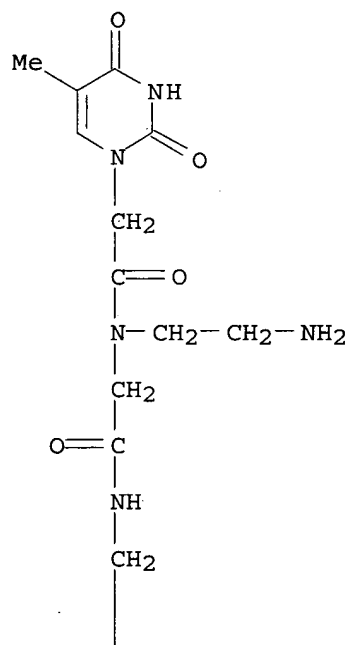
PAGE 1-C



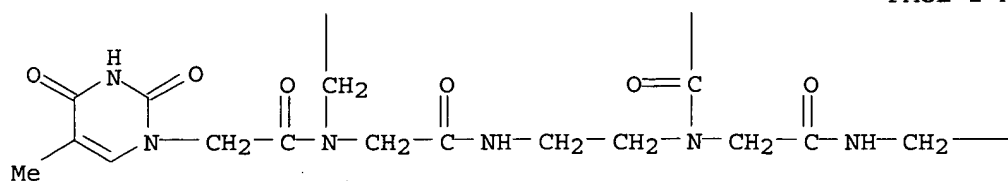
RN 695183-73-4 HCAPLUS

CN Peptide nucleic acid, (H-T-T-C-T-C-T-T-T)-Bal-OH (9CI) (CA INDEX NAME)

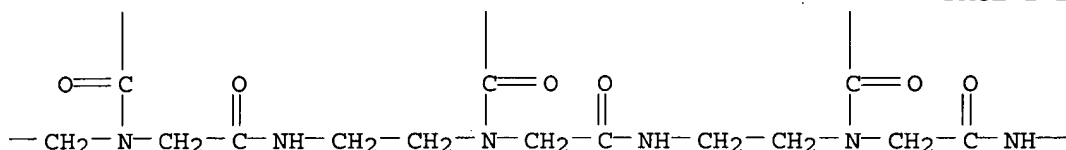
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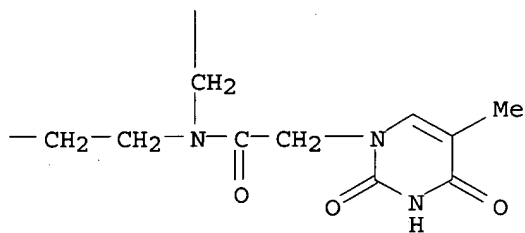
PAGE 2-A



PAGE 2-B



PAGE 2-C



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L38 ANSWER 3 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:731219 HCAPLUS

DOCUMENT NUMBER: 140:16951

TITLE: Expanding the repertoire of pyrrolidyl PNA analogues for DNA/RNA hybridization selectivity: aminoethylpyrrolidinone PNA (aepone-PNA)

AUTHOR(S): Sharma, Nagendra K.; Ganesh, Krishna N.

CORPORATE SOURCE: Division of Organic Chemistry (Synthesis), National Chemical Laboratory, Pune, 411008, India

SOURCE: Chemical Communications (Cambridge, United Kingdom) (2003), (19), 2484-2485

CODEN: CHCOFS; ISSN: 1359-7345

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:16951

AB New PNA analogs derived from aminoethylpyrrolidin-5-one backbone show stabilization of aepone-PNA:DNA hybrids and destabilization of the corresponding RNA hybrids compared to unmodified PNA.

CC 34-3 (Amino Acids, Peptides, and Proteins)

Section cross-reference(s): 3

IT 4005-49-6 10310-21-1 149411-91-6 65-71-4, Thymine

253307-68-5

RL: RCT (Reactant)

(expanding the repertoire of pyrrolidyl PNA analogs for DNA/RNA hybridization selectivity: aminoethylpyrrolidinone PNA (aepone-PNA))

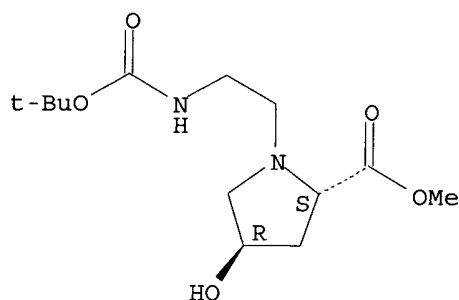
IT **340961-32-2P** 675824-96-1P 709028-76-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (expanding the repertoire of pyrrolidyl PNA analogs for DNA/RNA hybridization selectivity: aminoethylpyrrolidinone PNA (aepone-PNA))

IT **253307-86-7P 253342-13-1P** 631897-21-7P 631897-22-8P
 631897-23-9P 631897-24-0P **631897-25-1P 631897-26-2P**
 631897-27-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (expanding the repertoire of pyrrolidyl PNA analogs for DNA/RNA hybridization selectivity: aminoethylpyrrolidinone PNA (aepone-PNA))

IT **253307-68-5**
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (expanding the repertoire of pyrrolidyl PNA analogs for DNA/RNA hybridization selectivity: aminoethylpyrrolidinone PNA (aepone-PNA))

RN 253307-68-5 HCAPLUS
 CN L-Proline, 1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-4-hydroxy-, methyl ester, (4R)- (9CI) (CA INDEX NAME)

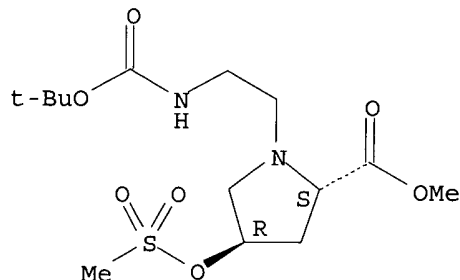
Absolute stereochemistry.



IT **340961-32-2P**
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (expanding the repertoire of pyrrolidyl PNA analogs for DNA/RNA hybridization selectivity: aminoethylpyrrolidinone PNA (aepone-PNA))

RN 340961-32-2 HCAPLUS
 CN L-Proline, 1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-4-[(methylsulfonyl)oxy]-, methyl ester, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



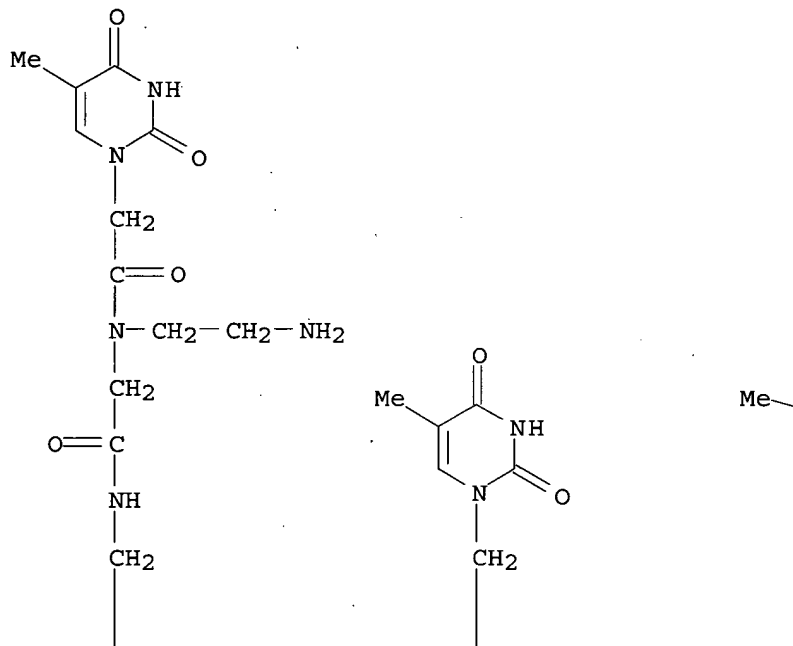
IT 253307-86-7P 253342-13-1P 631897-25-1P
631897-26-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(expanding the repertoire of pyrrolidyl PNA analogs for DNA/RNA
hybridization selectivity: aminoethylpyrrolidinone PNA (aepone-PNA))

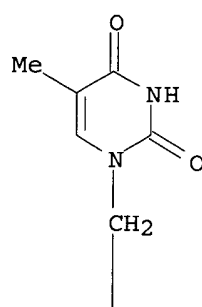
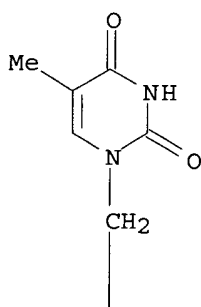
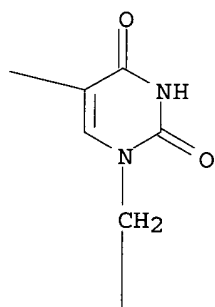
RN 253307-86-7 HCAPLUS

CN Peptide nucleic acid, (H-T-T-T-T-T-T-T)- β -ala-OH (9CI) (CA INDEX
NAME)

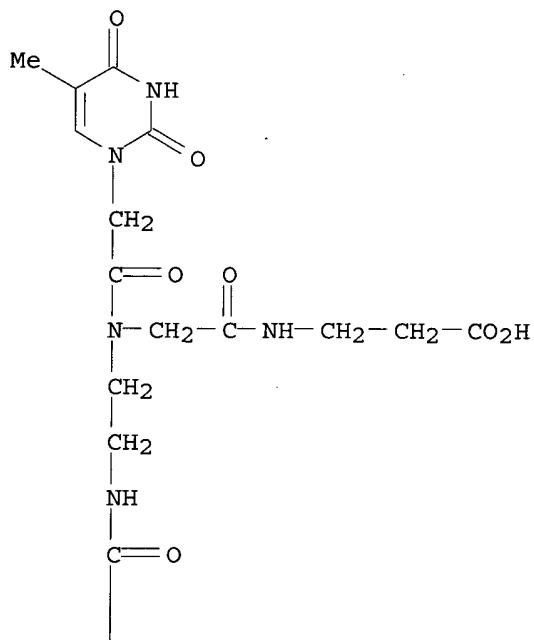
PAGE 1-A



PAGE 1-B



PAGE 1-C

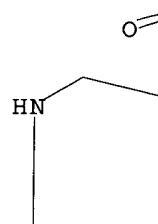


Cc1ccn(CCC(=O)NCCC(=O)NC(C)(C)CC(=O)NCCC(=O)NCCC(=O)NCCC(=O)N)c(=O)[nH]c1=O
$$\begin{array}{ccccccc} \begin{array}{c} | \\ \text{O}=\text{C} \\ | \end{array} & & & & \begin{array}{c} | \\ \text{C}=\text{O} \\ | \end{array} & & \begin{array}{c} | \\ \text{C}=\text{O} \\ | \end{array} \\ -\text{CH}_2-\text{N}-\text{CH}_2-\text{C}(=\text{O})-\text{NH}-\text{CH}_2-\text{CH}_2-\text{N}-\text{CH}_2-\text{C}(=\text{O})-\text{NH}-\text{CH}_2-\text{CH}_2-\text{N}-\text{CH}_2-\text{C}(=\text{O})-\text{NH}- & & & & & & \end{array}$$
CC1=CC(=O)NC(=O)N1CC(=O)N(C)CC[illegible]

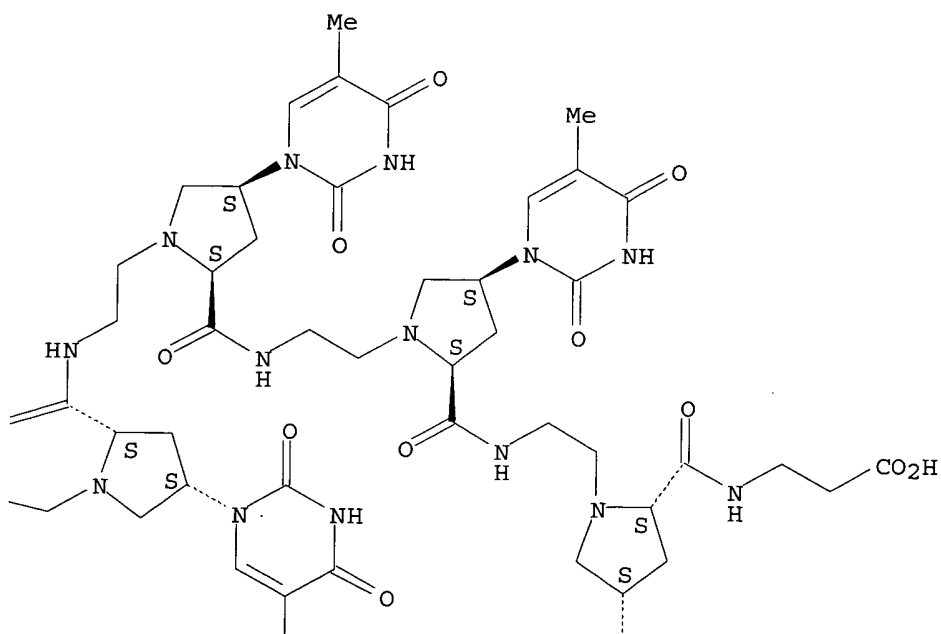
Page 77

PAGE 1-A

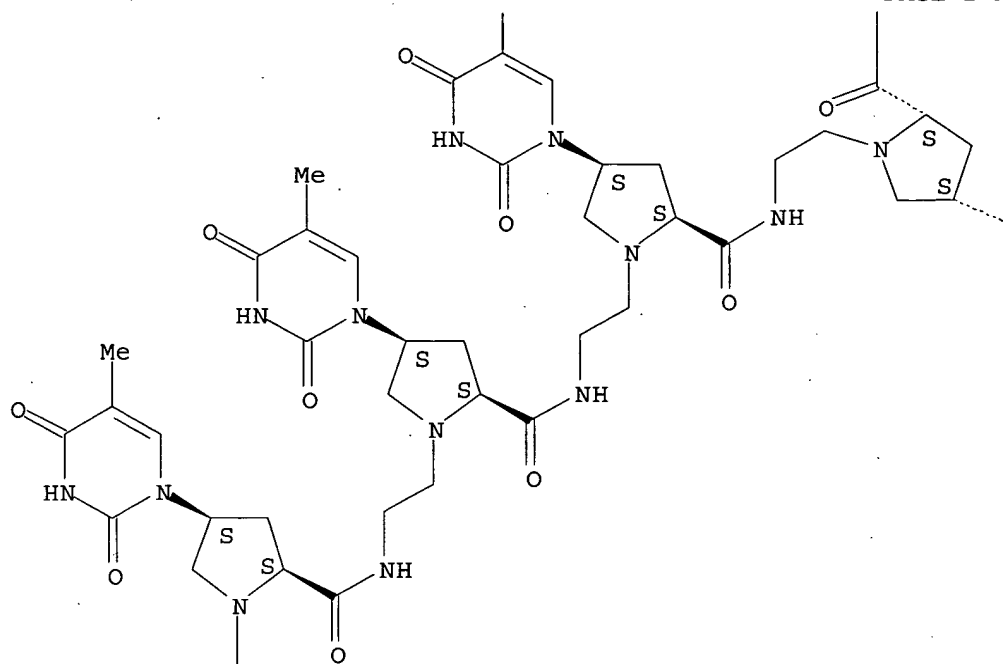
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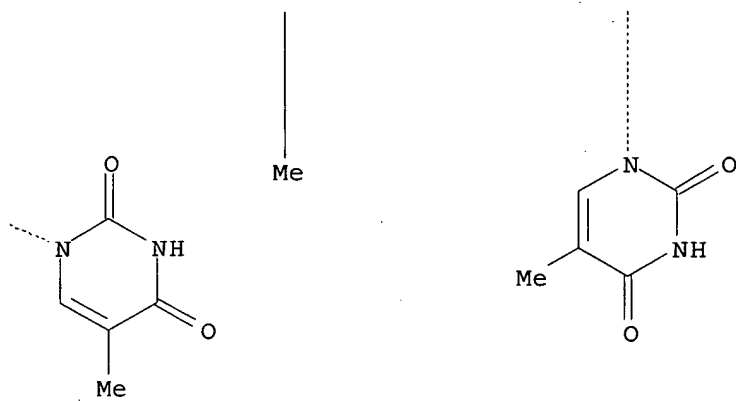
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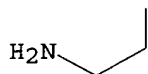
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PAGE 2-B



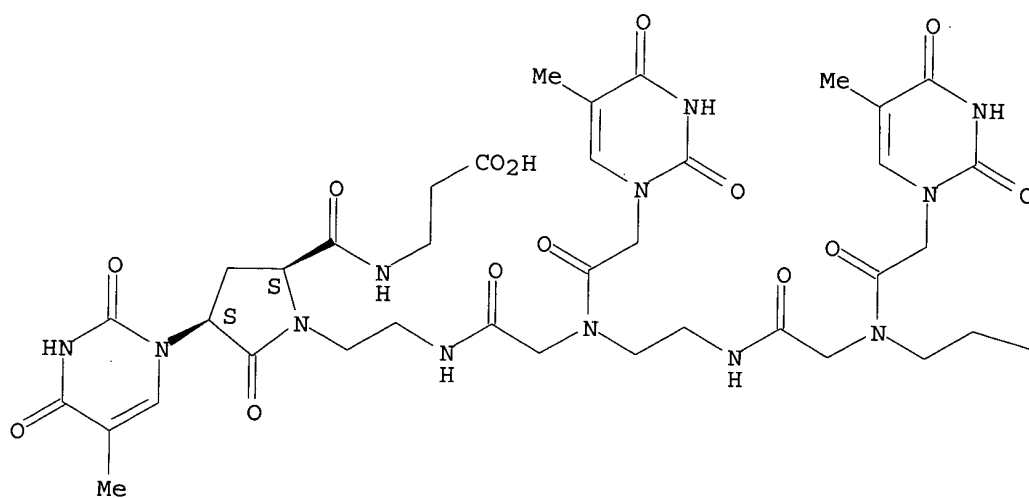
PAGE 3-A



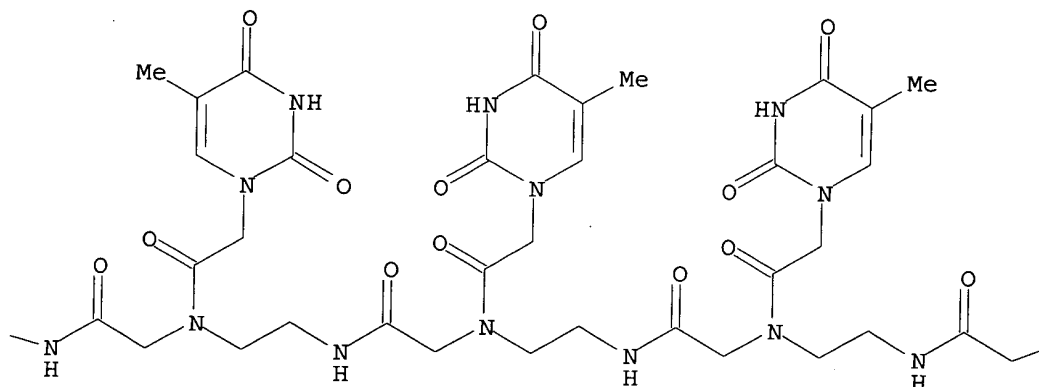
RN 631897-25-1 HCAPLUS
 CN Peptide nucleic acid, (H-T-T-T-T-T-T-T)-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-5-oxo-Pro-Bal-OH (9CI) (CA INDEX NAME)

Absolute stereochemistry.

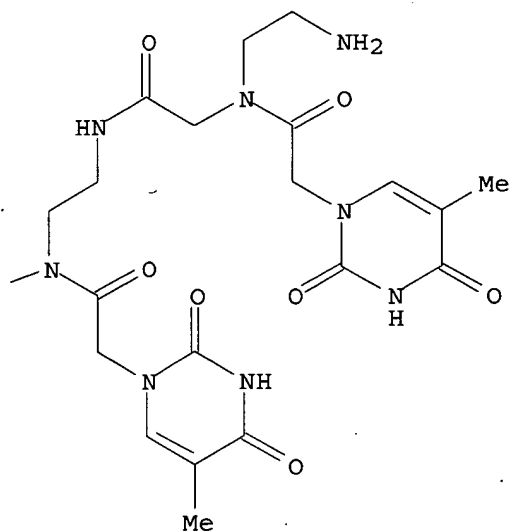
PAGE 1-A



PAGE 1-B



PAGE 1-C

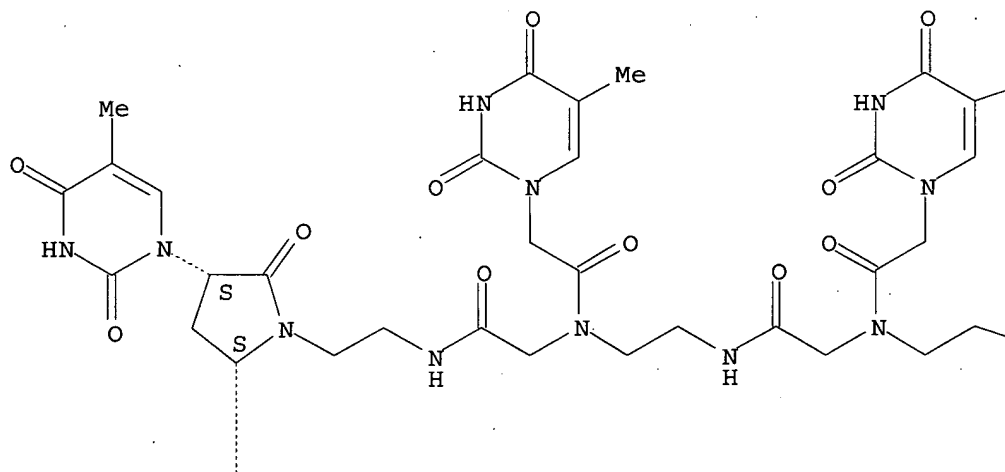


RN 631897-26-2 HCAPLUS

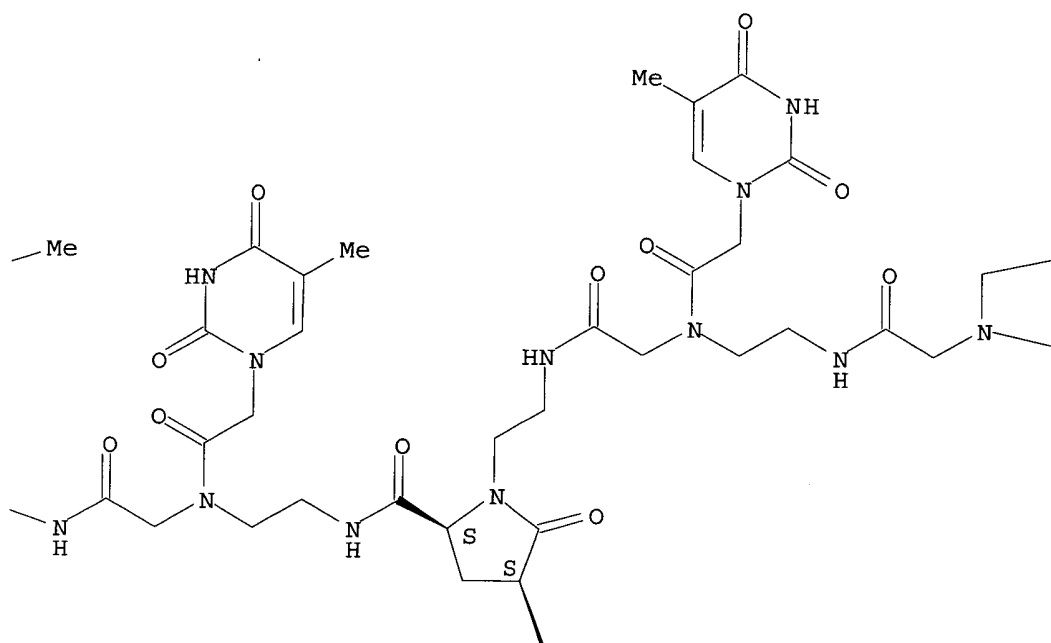
CN Peptide nucleic acid, (H-T-T-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-5-oxo-Pro-T-T-T)-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-5-oxo-Pro-Bal-OH (9CI) (CA INDEX NAME)

Absolute stereochemistry.

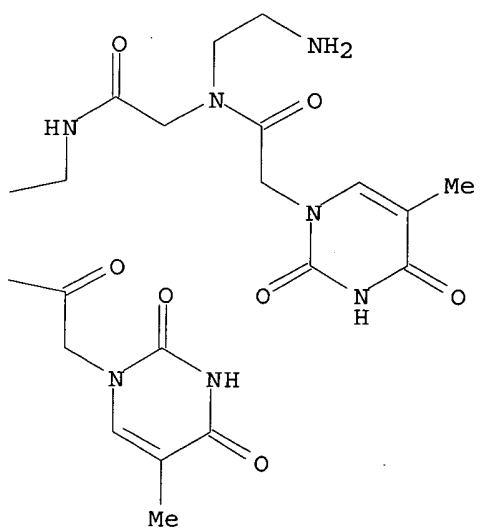
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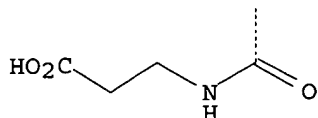
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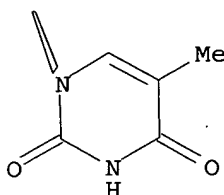
PAGE 1-C



PAGE 2-A



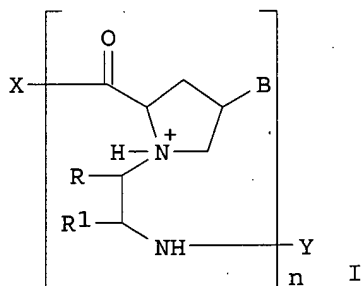
PAGE 2-B



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L38 ANSWER 4 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 2003:678488 HCAPLUS
 DOCUMENT NUMBER: 139:214718
 TITLE: Chiral peptide nucleic acids with a
 N-aminoethyl-D-proline backbone
 INVENTOR(S): Lowe, Gordon
 PATENT ASSIGNEE(S): Isis Innovation Ltd., UK
 SOURCE: U.S. Pat. Appl. Publ., 14 pp.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003162699	A1	20030828	US 2001-22585	20011030
US 6716961	B2	20040406		
PRIORITY APPLN. INFO.:			US 2001-22585	20011030
OTHER SOURCE(S):	MARPAT 139:214718			
GI				



AB Chiral peptide nucleic acids are provided which hybridize strongly with

complementary nucleic acids and have potential as antigene and antisense agents and as tools in mol. biol. The compds. have formula I [n is 1-200; B is an (un)protected base; X is OH or OR₂, where R₂ is a protecting, activating, or lipophilic group, an amino acid, amino amide, or nucleoside; Y is H or a protecting, lipophilic, or aminoacyl group or a nucleoside; R, R₁ are H, alkyl, aryl, or aralkyl or may form a cycloalkyl ring]. Thus, H-[(Ψ-CH₂)Gly-D-Pro(T)]₁₀-Lys-NH₂ was prepared and complexed with oligonucleotides [T_m = 53° for complex with poly(rA)].

IC ICM A61K038-16
ICS A61K031-52; C07K014-00

INCL 514012000; 514013000; 514014000; 514015000; 514016000; 514017000;
514018000; 514263200; 544277000; 544266000

CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 6, 33

IT **586954-19-0P**
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of chiral peptide nucleic acids with N-aminoethyl-D-proline backbone and hybridization with oligonucleotides)

IT **586954-21-4P 586954-37-2P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation of chiral peptide nucleic acids with N-aminoethyl-D-proline backbone and hybridization with oligonucleotides)

IT 18226-05-6P 43090-97-7P 318515-52-5P **318515-53-6P**
318515-54-7P 318515-55-8P **318515-56-9P** 586954-18-9P
586954-22-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of chiral peptide nucleic acids with N-aminoethyl-D-proline backbone and hybridization with oligonucleotides)

IT **586954-19-0P**
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of chiral peptide nucleic acids with N-aminoethyl-D-proline backbone and hybridization with oligonucleotides)

RN 586954-19-0 HCAPLUS

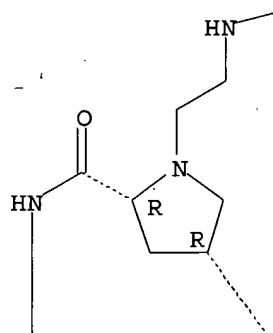
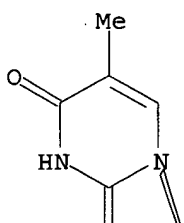
CN Peptide nucleic acid, (H-[(4R)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro]₁₀-Lys-NH₂ (9CI) (CA INDEX NAME)

Absolute stereochemistry.

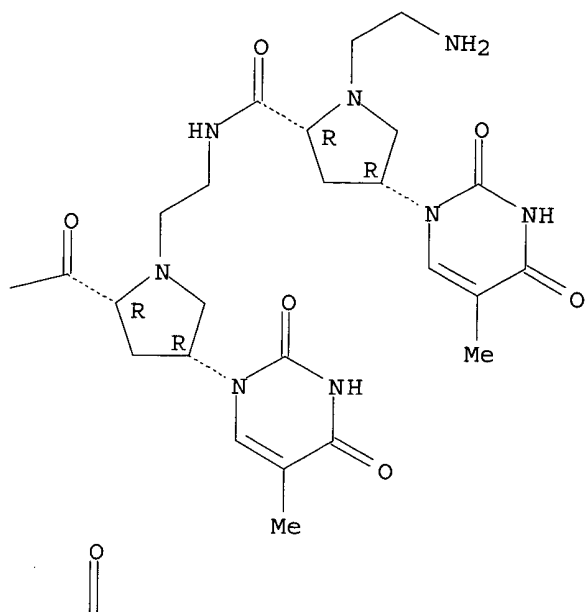
PAGE 1-A

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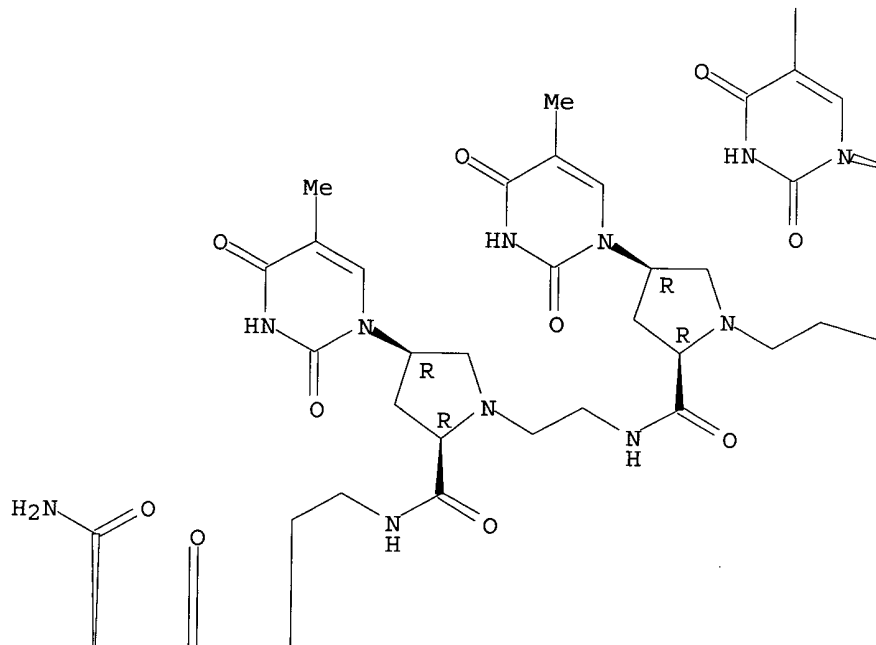
PAGE 1-B



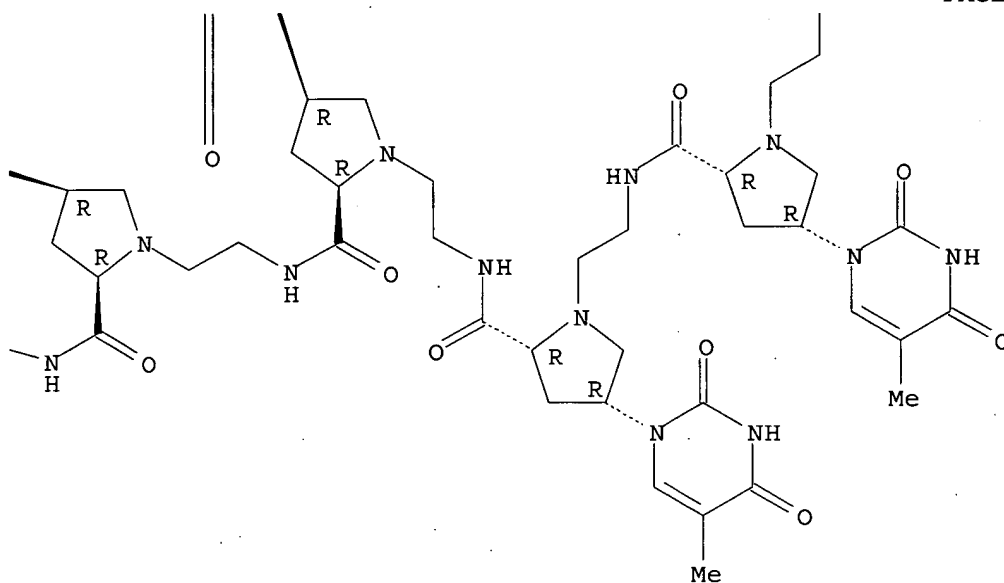
PAGE 1-C



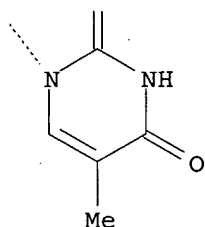
PAGE 2-A



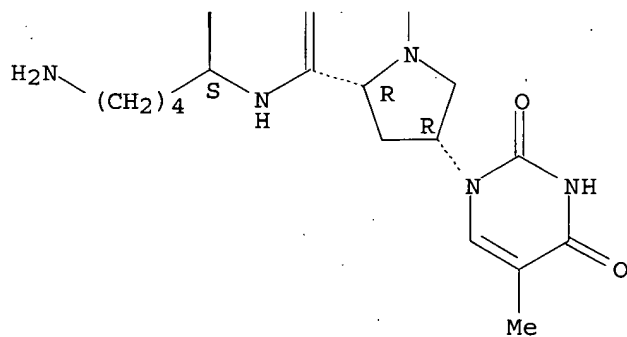
PAGE 2-B



PAGE 2-C



PAGE 3-A



IT 586954-21-4P 586954-37-2P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (preparation of chiral peptide nucleic acids with N-aminoethyl-D-proline
 backbone and hybridization with oligonucleotides)

RN 586954-21-4 HCAPLUS

CN 5'-Adenylic acid, homopolymer, complex with peptide nucleic acid
(H-[(4R)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-
pyrimidinyl)-D-Pro]10)-Lys-NH2 (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 586954-19-0

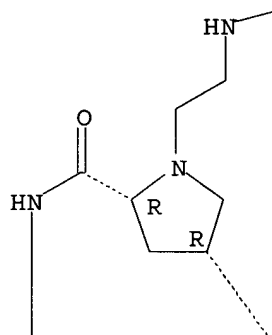
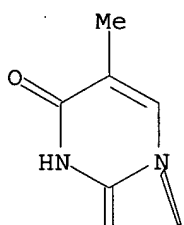
CMF C126 H175 N43 O31

Absolute stereochemistry.

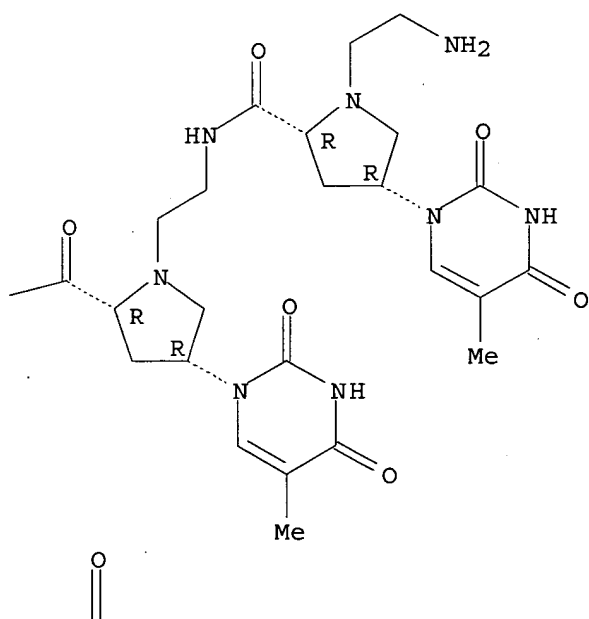
PAGE 1-A

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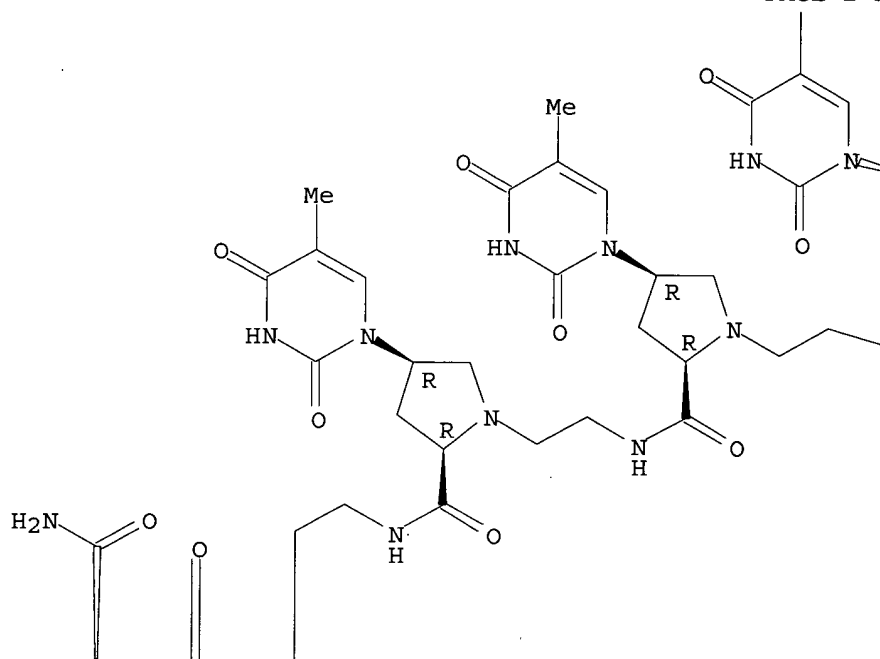
PAGE 1-B



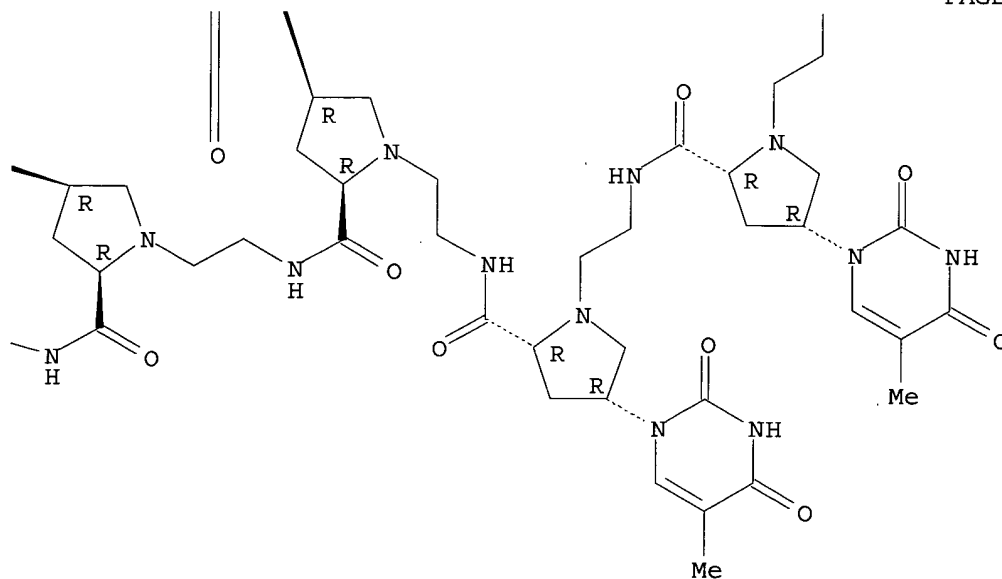
PAGE 1-C



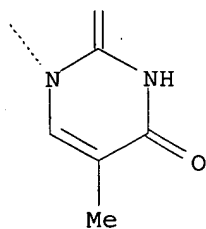
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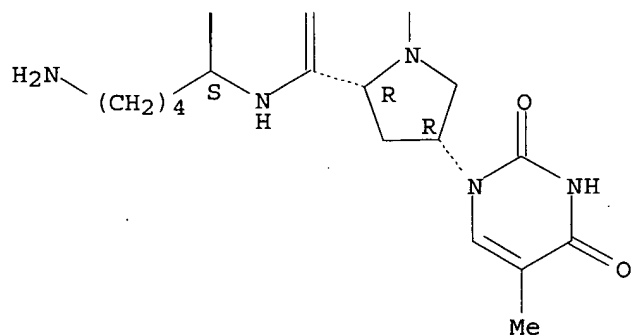
PAGE 2-B



PAGE 2-C



PAGE 3-A



CM 2

CRN 24937-83-5

CMF (C10 H14 N5 O7 P)x

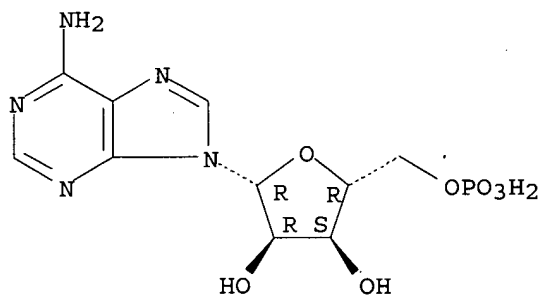
CCI PMS

CM 3

CRN 61-19-8

CMF C10 H14 N5 O7 P

Absolute stereochemistry.



RN 586954-37-2 HCAPLUS

CN 5'-Adenylic acid, 2'-deoxy-, homopolymer, complex with peptide nucleic acid (H-[(4R)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro]10)-Lys-NH2 (1:1) (9CI) (CA INDEX NAME)

CM 1

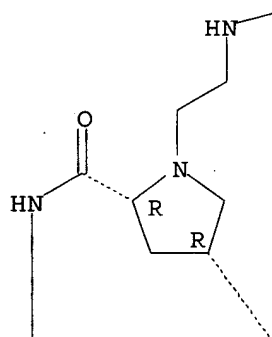
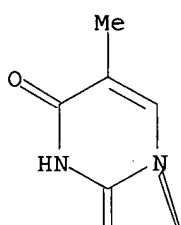
CRN 586954-19-0
CMF C126 H175 N43 O31

Absolute stereochemistry.

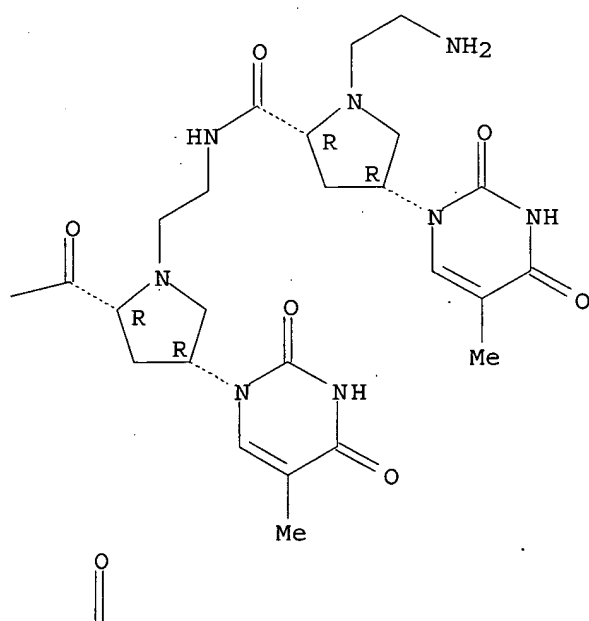
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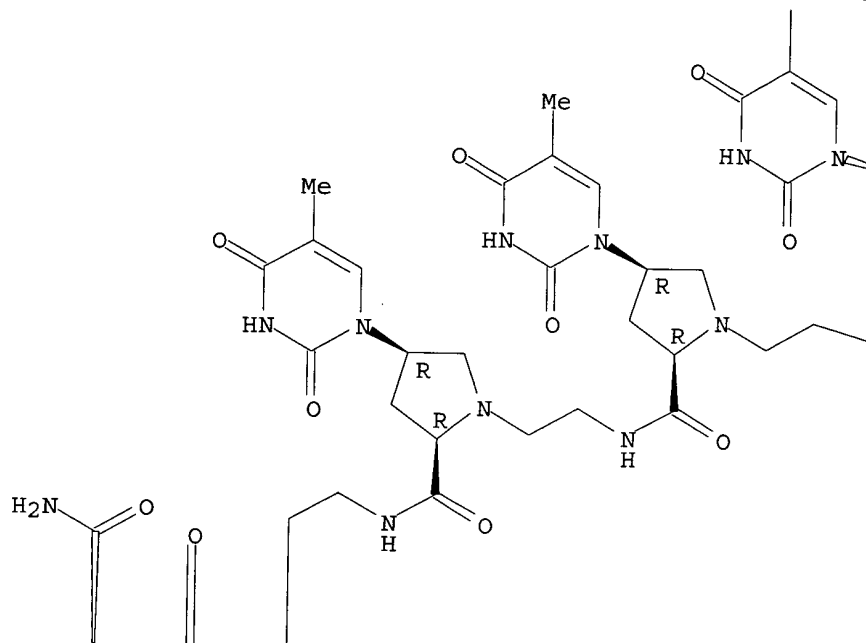
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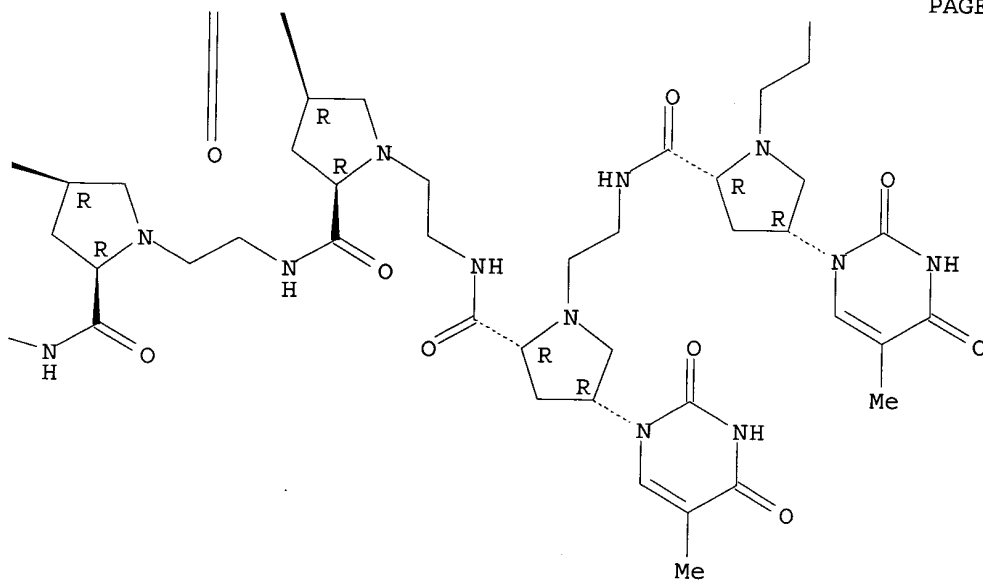
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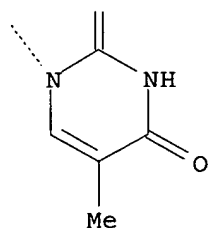
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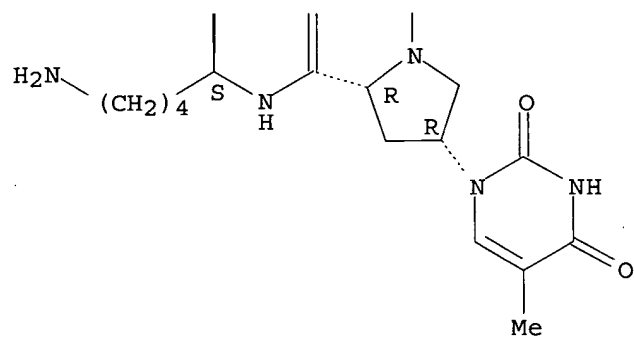
PAGE 2-B



PAGE 2-C



PAGE 3-A



CM 2

CRN 25191-20-2

CMF (C10 H14 N5 O6 P)x

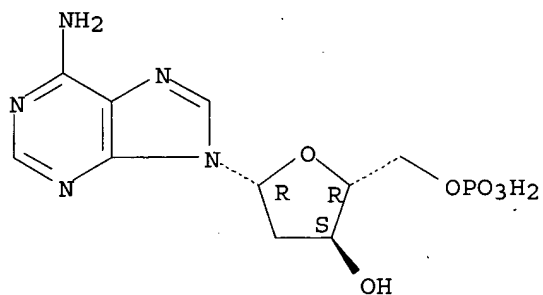
CCI PMS

CM 3

CRN 653-63-4

CMF C10 H14 N5 O6 P

Absolute stereochemistry. Rotation (+).



IT 318515-53-6P 318515-56-9P

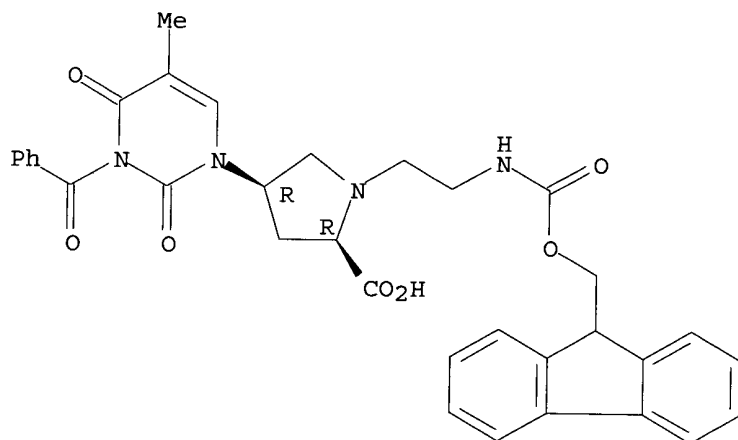
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of chiral peptide nucleic acids with N-aminoethyl-D-proline

backbone and hybridization with oligonucleotides)

RN 318515-53-6 HCAPLUS
 CN D-Proline, 4-(3-benzoyl-3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-1-[2-[[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]ethyl]-, monohydrochloride, (4R)-(9CI) (CA INDEX NAME)

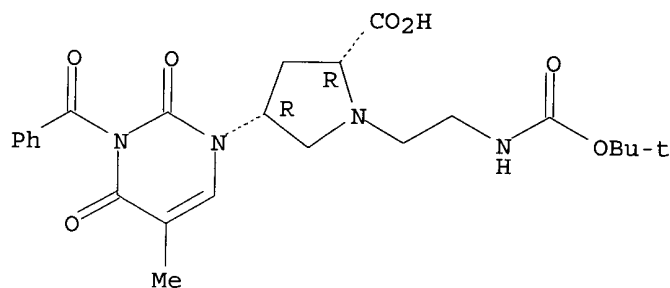
Absolute stereochemistry. Rotation (+).



● HCl

RN 318515-56-9 HCAPLUS
 CN D-Proline, 4-(3-benzoyl-3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, (4R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L38 ANSWER 5 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:625327 HCAPLUS

DOCUMENT NUMBER: 139:373791

TITLE: Design and synthesis of **fluorescent** β -cyclodextrins for the enantioselective sensing of α -amino acids

AUTHOR(S): Corradini, R.; Paganuzzi, C.; Marchelli, R.; Pagliari, S.; Sforza, S.; Dossena, A.; Galaverna, G.; Duchateau, A.
 CORPORATE SOURCE: Dipartimento di Chimica Organica e Industriale, Parma, Italy
 SOURCE: Chirality (2003), 15(Suppl.), S30-S39
 CODEN: CHRLEP; ISSN: 0899-0042
 PUBLISHER: Wiley-Liss, Inc.
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB **Fluorescent** monofunctionalized β -cyclodextrins bearing a copper(II) binding side arm and a dansyl group (CD-NH-AA-CH₂CH₂NH-DNS) were designed as enantioselective sensors for unmodified α -amino acids. The side arm was derived from amino acid synthons (AA = L- and D-phenylalanine (1 and 2), L- and D-phenylglycine (3 and 4), L-proline (5), and L-cyclohexylglycine (6)) and was chosen to contain an amide, an amine, and a sulfonamide group. Enantioselectivity was evaluated by addition of copper(II) complexes of D- or L-valine and D- or L-proline. Chiral discrimination in the **fluorescence** response was observed in all cases, due to a ligand exchange process. The best conditions for these expts. are the use of an excess (10:1) of the copper complex. The cyclodextrin 4 containing a D-phenylglycine unit is poorly enantioselective, as found for 2, suggesting that the best design can be obtained by using L-amino acids. All L-amino acid containing cyclodextrins showed good enantioselectivities, some of which were higher than those already reported for 1. Other analytes related to amino acids were studied using cyclodextrins 1 and 3. Enantiomers of α,α -disubstituted amino acids, N-methylamino acids, and amino acid amides are discriminated, while β -phenylalanine and other mols. bearing a poor anchoring group at the α -carbon gave poor enantioselectivity. From the present data a model for the recognition process, based on the formation of ternary diastereomeric complexes, is proposed.

CC 80-3 (Organic Analytical Chemistry)

ST **fluorescent** beta cyclodextrin prepn amino acid enantioselective sensing

IT Amino acids, analysis

RL: ANT (Analyte); ANST (Analytical study)
 (analytes; design and synthesis of **fluorescent** β -cyclodextrins for the enantioselective sensing of α -amino acids)

IT Chiral recognition
 Fluorometry

(design and synthesis of **fluorescent** β -cyclodextrins for the enantioselective sensing of α -amino acids)

IT 97-69-8 565-07-1 614-19-7 700-63-0 875-74-1 1115-69-1
 2018-61-3 2566-30-5 2566-35-0 2835-06-5 2901-75-9 2935-35-5
 4540-60-7 6485-52-5 6485-67-2 10172-89-1 13398-26-0 13474-14-1
 13921-90-9 19436-52-3 29738-09-8 32526-16-2 40856-44-8
 54896-58-1 54896-65-0 56564-52-4 90899-85-7

RL: ANT (Analyte); ANST (Analytical study)
 (analyte; design and synthesis of **fluorescent** β -cyclodextrins for the enantioselective sensing of α -amino acids)

IT 620176-27-4P 620176-28-5P 620176-29-6P 620176-30-9P
 RL: ARG (Analytical reagent use); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
 (design and synthesis of **fluorescent** β -cyclodextrins for the enantioselective sensing of α -amino acids)

IT 289491-88-9

RL: ARU (Analytical role, unclassified); NUU (Other use, unclassified);
ANST (Analytical study); USES (Uses)

(design and synthesis of **fluorescent** β -cyclodextrins for
the enantioselective sensing of α -amino acids)

IT 289491-90-3

RL: ARU (Analytical role, unclassified); NUU (Other use, unclassified);

PRP (Properties); ANST (Analytical study); USES (Uses)

(design and synthesis of **fluorescent** β -cyclodextrins for
the enantioselective sensing of α -amino acids)

IT 7440-50-8, Copper, uses

RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)

(divalent; in enantioselective sensing of α -amino acids using
preparation of **fluorescent** β -cyclodextrins)

IT 620176-49-0P 620176-50-3P 620176-51-4P 620176-53-6P 620176-54-7P

620176-55-8P **620176-56-9P** 620176-57-0P 620176-58-1P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)

(in preparation of **fluorescent** β -cyclodextrins for the
enantioselective sensing of α -amino acids)

IT 605-65-2, Dansyl chloride 41324-66-7 66190-91-8 68745-09-5

89711-08-0 115937-23-0 620176-48-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(in preparation of **fluorescent** β -cyclodextrins for the
enantioselective sensing of α -amino acids)

IT 620176-59-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

(in preparation of **fluorescent** β -cyclodextrins for the
enantioselective sensing of α -amino acids)

IT **620176-56-9P**

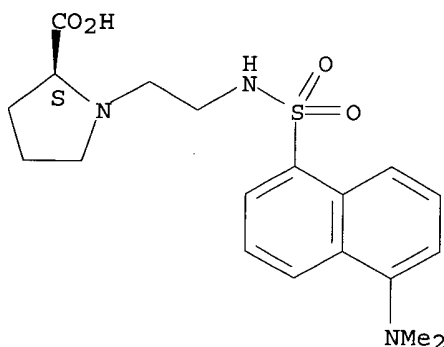
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)

(in preparation of **fluorescent** β -cyclodextrins for the
enantioselective sensing of α -amino acids)

RN 620176-56-9 HCAPLUS

CN L-Proline, 1-[2-[[[5-(dimethylamino)-1-naphthalenyl]sulfonyl]amino]ethyl]-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L38 ANSWER 6 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:347055 HCAPLUS

DOCUMENT NUMBER: 139:80857

TITLE: N7-Guanine as a C+ mimic in hairpin aeg/aepPNA-DNA triplex: Probing binding selectivity by UV-Tm and kinetics by **fluorescence**-based strand-invasion assay

AUTHOR(S): D'Costa, Moneesha; Kumar, Vaijayanti A.; Ganesh, Krishna N.

CORPORATE SOURCE: Division of Organic Chemistry (Synthesis), National Chemical Laboratory, Pune, 411008, India

SOURCE: Journal of Organic Chemistry (2003), 68(11), 4439-4445
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:80857

AB N7-substituted guanine (N7G) has been introduced into aminoethylglycyl bisPNA as a C+ mimic to achieve pH-independent triplex formation with complementary DNA sequences. The introduction of chiral, cationic aminoethylprolyl units with C+ and C+ mimic N7G in the backbone of bisPNAs influenced the recognition of cDNA in an orientation-selective manner. A simple **fluorescence** assay is developed to examine the process of strand invasion of target DNA duplex by these modified bisPNAs and comparative results of the study employing triplex forming polypyrimidine (C/T) and purine-pyrimidine mixmer-bisPNAs are presented.

CC 6-2 (General Biochemistry)
Section cross-reference(s): 33

IT Quaternary structure
(DNA triplex; N7-guanine as a C+ mimic in hairpin aminoethylglycyl/aminoethylprolylpeptide nucleic acid-DNA triplex based on probing binding selectivity by UV-Tm and kinetics by **fluorescence**-based strand-invasion assay)

IT Nucleic acid hybridization
(N7-guanine as a C+ mimic in hairpin aminoethylglycyl/aminoethylprolylpeptide nucleic acid-DNA triplex based on probing binding selectivity by UV-Tm and kinetics by **fluorescence**-based strand-invasion assay)

IT Peptide nucleic acids
RL: PEP (Physical, engineering or chemical process); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(N7-guanine as a C+ mimic in hairpin aminoethylglycyl/aminoethylprolylpeptide nucleic acid-DNA triplex based on probing binding selectivity by UV-Tm and kinetics by **fluorescence**-based strand-invasion assay)

IT DNA
RL: PEP (Physical, engineering or chemical process); PYP (Physical process); PROC (Process)
(double-stranded; N7-guanine as a C+ mimic in hairpin aminoethylglycyl/aminoethylprolylpeptide nucleic acid-DNA triplex based on probing binding selectivity by UV-Tm and kinetics by **fluorescence**-based strand-invasion assay)

IT 552898-84-7P 552898-85-8P 552898-86-9P 552898-87-0P
RL: PEP (Physical, engineering or chemical process); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(N7-guanine as a C+ mimic in hairpin aminoethylglycyl/aminoethylprolylpeptide nucleic acid-DNA triplex based on probing binding selectivity by UV-Tm and kinetics by **fluorescence**-based strand-invasion assay)

IT 21047-89-2 72648-80-7 172729-74-7 253307-68-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(N7-guanine as a C+ mimic in hairpin aminoethylglycyl/aminoethylprolylpeptide nucleic acid-DNA triplex based on probing binding selectivity by UV-Tm and kinetics by **fluorescence**-based strand-invasion assay)

ptide nucleic acid-DNA triplex based on probing binding selectivity by UV-Tm and kinetics by **fluorescence**-based strand-invasion assay)

IT 169566-58-9P 340961-32-2P 340961-34-4P
340961-45-7P 552333-54-7P 552333-55-8P
552333-56-9P 552333-57-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(N7-guanine as a C+ mimic in hairpin aminoethylglycyl/aminoethylprolylpeptide nucleic acid-DNA triplex based on probing binding selectivity by UV-Tm and kinetics by **fluorescence**-based strand-invasion assay)

IT 253307-68-5

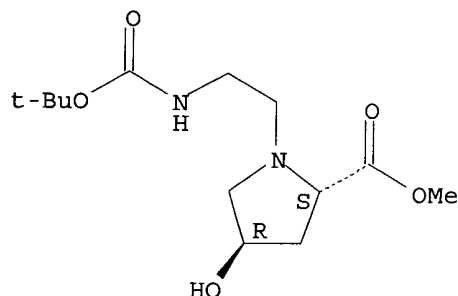
RL: RCT (Reactant); RACT (Reactant or reagent)

(N7-guanine as a C+ mimic in hairpin aminoethylglycyl/aminoethylprolylpeptide nucleic acid-DNA triplex based on probing binding selectivity by UV-Tm and kinetics by **fluorescence**-based strand-invasion assay)

RN 253307-68-5 HCAPLUS

CN L-Proline, 1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-4-hydroxy-, methyl ester, (4R) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.



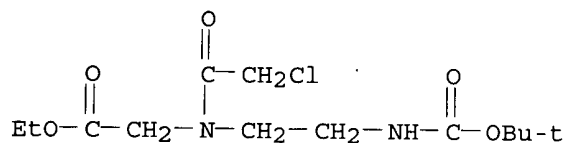
IT 169566-58-9P 340961-32-2P 340961-34-4P
340961-45-7P 552333-54-7P 552333-55-8P
552333-56-9P 552333-57-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(N7-guanine as a C+ mimic in hairpin aminoethylglycyl/aminoethylprolylpeptide nucleic acid-DNA triplex based on probing binding selectivity by UV-Tm and kinetics by **fluorescence**-based strand-invasion assay)

RN 169566-58-9 HCAPLUS

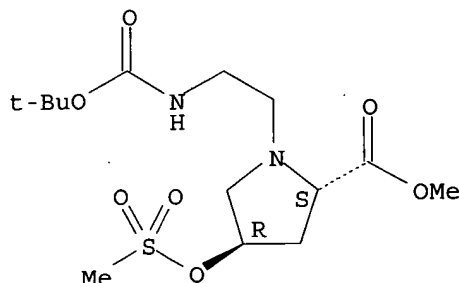
CN Glycine, N-(chloroacetyl)-N-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 340961-32-2 HCAPLUS

CN L-Proline, 1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-4-
[(methylsulfonyl)oxy]-, methyl ester, (4R)- (9CI) (CA INDEX NAME)

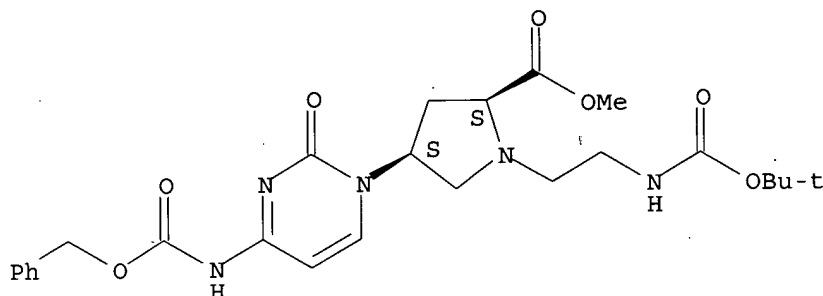
Absolute stereochemistry.



RN 340961-34-4 HCAPLUS

CN L-Proline, 1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-4-[2-oxo-4-
[[[phenylmethoxy]carbonyl]amino]-1(2H)-pyrimidinyl]-, methyl ester, (4S)-
(9CI) (CA INDEX NAME)

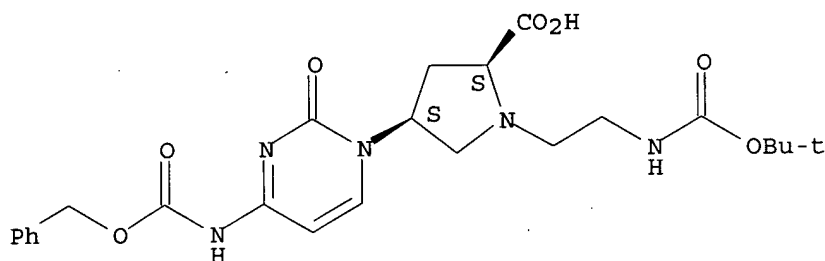
Absolute stereochemistry.



RN 340961-45-7 HCAPLUS

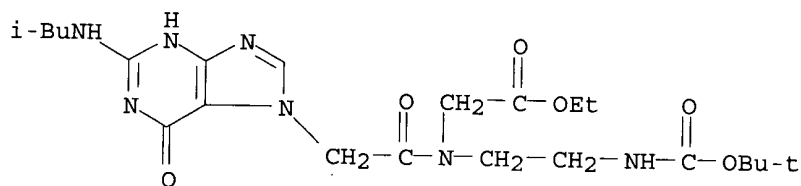
CN L-Proline, 1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-4-[2-oxo-4-
[[[phenylmethoxy]carbonyl]amino]-1(2H)-pyrimidinyl]-, (4S)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.



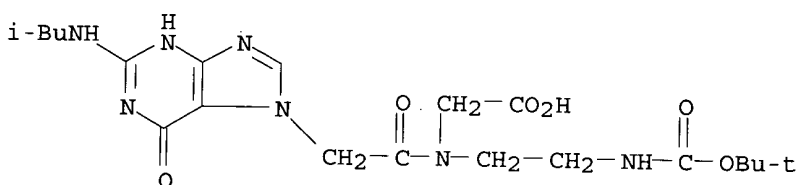
RN 552333-54-7 HCAPLUS

CN Glycine, N-[[[1,6-dihydro-2-[(2-methylpropyl)amino]-6-oxo-7H-purin-7-
yl]acetyl]-N-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, ethyl ester
(9CI) (CA INDEX NAME)



RN 552333-55-8 HCAPLUS

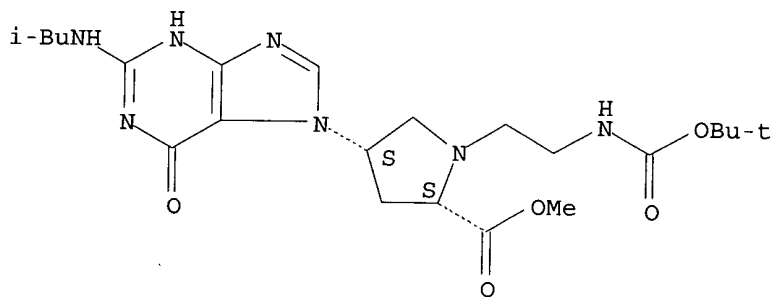
CN Glycine, N-[[1,6-dihydro-2-[(2-methylpropyl)amino]-6-oxo-7H-purin-7-yl]acetyl]-N-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]- (9CI) (CA INDEX NAME)



RN 552333-56-9 HCAPLUS

CN L-Proline, 4-[1,6-dihydro-2-[(2-methylpropyl)amino]-6-oxo-7H-purin-7-yl]-1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, methyl ester, (4S)- (9CI) (CA INDEX NAME)

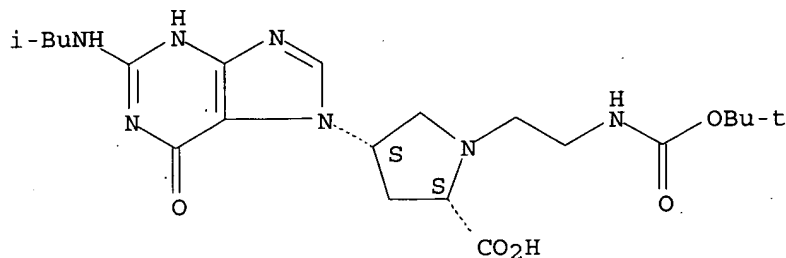
Absolute stereochemistry.



RN 552333-57-0 HCAPLUS

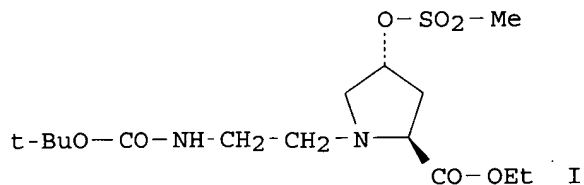
CN L-Proline, 4-[1,6-dihydro-2-[(2-methylpropyl)amino]-6-oxo-7H-purin-7-yl]-1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L38 ANSWER 7 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 2001:710917 HCAPLUS
 DOCUMENT NUMBER: 136:216993
 TITLE: Synthesis and binding affinity of a chiral PNA analogue
 AUTHOR(S): Li, Ying; Jin, Tao; Liu, Keliang
 CORPORATE SOURCE: Beijing Institute of Pharmacology and Toxicology, Beijing, 100850, Peop. Rep. China
 SOURCE: Nucleosides, Nucleotides & Nucleic Acids (2001), 20(9), 1705-1721
 CODEN: NNNAFY; ISSN: 1525-7770
 PUBLISHER: Marcel Dekker, Inc.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB The synthesis of a chiral peptide nucleic acid (PNA), which is composed of N-aminoethyl-cis-4-nucleobase-L-proline units, was described. The chiral PNA monomers containing all four nucleobases (A, T, C and G) were stereoselectively prepared using key intermediate (I), prepared in two steps from (CH₃)₃COC(O)NH(CH₂)₂Br and trans-L-hydroxyproline Et ester hydrochloride. The x-ray diffraction data from a single crystal confirmed the configuration of a key intermediate. Binding activity of the oligomers with their complementary DNA targets was also investigated.

CC 33-10 (Carbohydrates)
 Section cross-reference(s): 6, 34

IT 386212-22-2P 386212-24-4P 401983-42-4P 401983-43-5P
 401983-44-6P 401983-45-7P 401983-46-8P 401983-47-9P 401983-48-0P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (preparation of cis-L-proline-based PNA oligomers and their hybridization characteristics with DNA)

IT 253307-71-0P 340961-43-5P 340961-45-7P
 371970-41-1P 386212-11-9P 386212-12-0P 386212-13-1P
 386212-14-2P 386212-15-3P 386212-16-4P 386212-17-5P 386212-18-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation of cis-L-proline-based PNA oligomers and their hybridization
characteristics with DNA)

IT 386212-19-7P 386212-20-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of cis-L-proline-based PNA oligomers and their hybridization
characteristics with DNA)

IT 386212-22-2P 386212-24-4P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation of cis-L-proline-based PNA oligomers and their hybridization
characteristics with DNA)

RN 386212-22-2 HCAPLUS

CN Adenosine, 2'-deoxyadenylyl-(3'→5')-thymidylyl-2'-deoxyadenylyl-
(3'→5')-thymidylyl-(3'→5')-thymidylyl-(3'→5')-
thymidylyl-(3'→5')-2'-deoxyadenylyl-(3'→5')-2'-deoxy-,
complex with peptide nucleic acid (H-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-
5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-L-prolyl-(4S)-1-(2-aminoethyl)-4-(6-
amino-9H-purin-9-yl)-L-prolyl-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-
methyl-2,4-dioxo-1(2H)-pyrimidinyl)-L-prolyl-(4S)-1-(2-aminoethyl)-4-(6-
amino-9H-purin-9-yl)-L-prolyl-(4S)-1-(2-aminoethyl)-4-(6-amino-9H-purin-9-
yl)-L-prolyl-(4S)-1-(2-aminoethyl)-4-(6-amino-9H-purin-9-yl)-L-prolyl-(4S)-
1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-L-
prolyl-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-
pyrimidinyl)-L-prolyl)-Lys-NH2 (1:1) (9CI) (CA INDEX NAME)

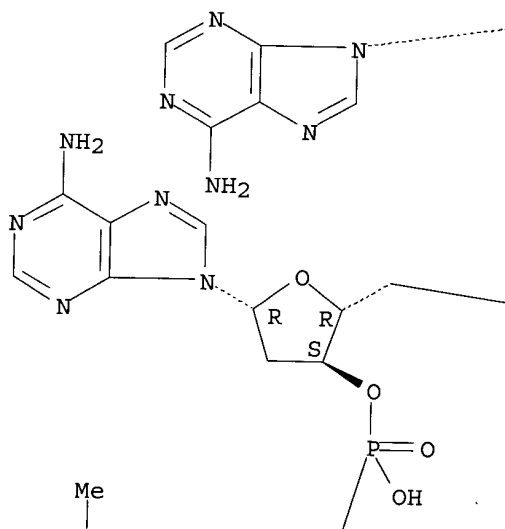
CM 1

CRN 386212-21-1

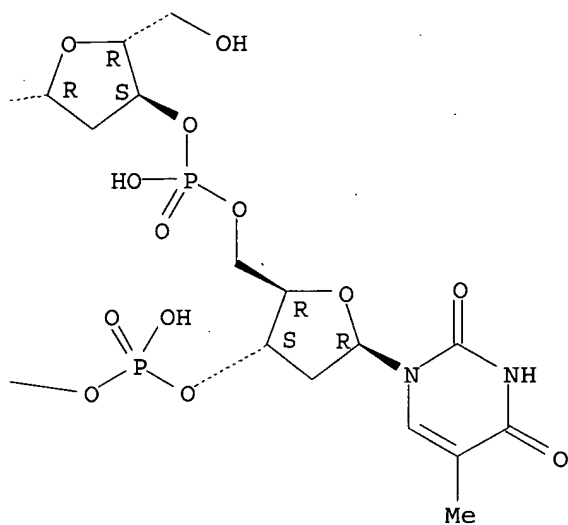
CMF C80 H101 N28 O46 P7

Absolute stereochemistry.

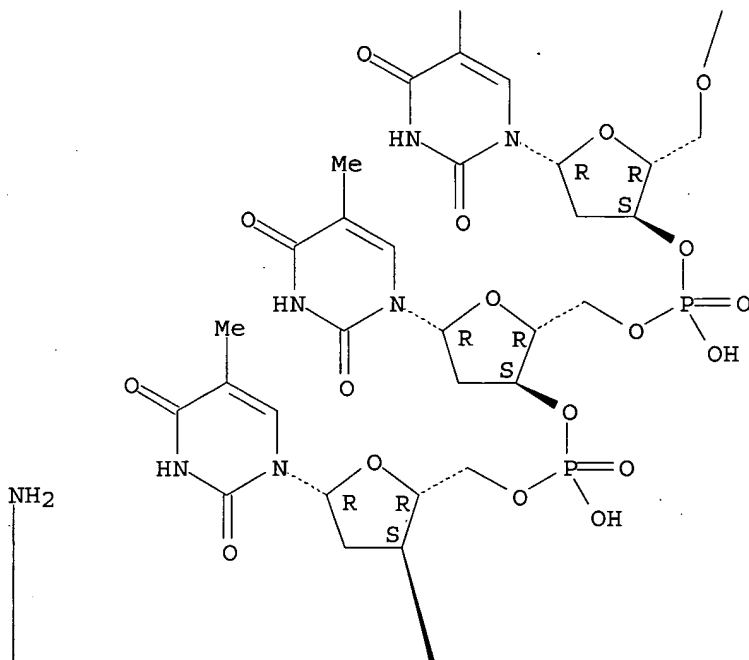
PAGE 1-A



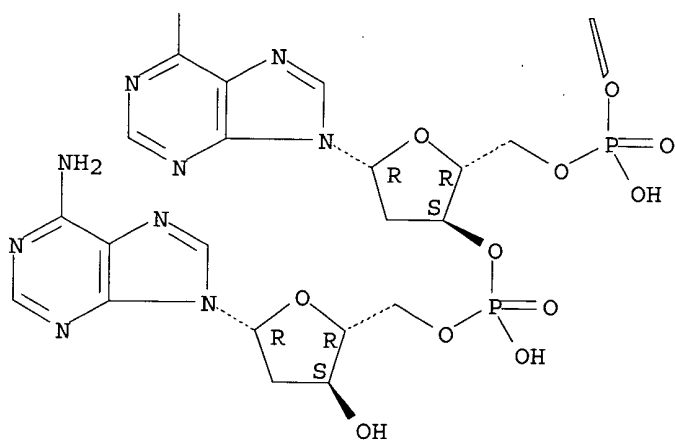
PAGE 1-B



PAGE 2-A



PAGE 3-A



CM 2

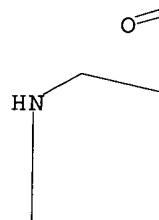
CRN 386212-19-7

CMF C102 H139 N47 O17

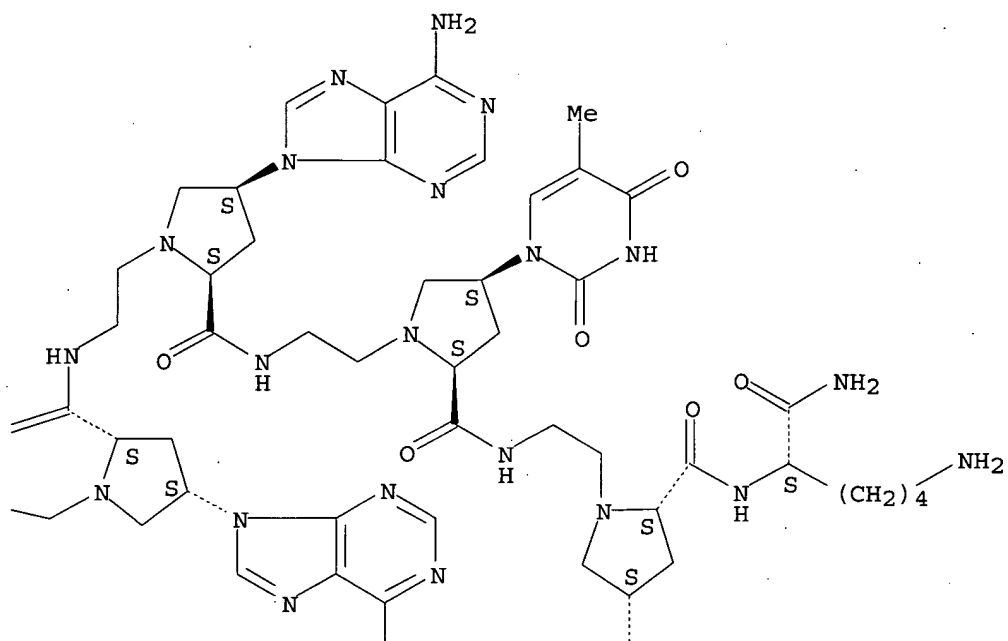
Absolute stereochemistry.

PAGE 1-A

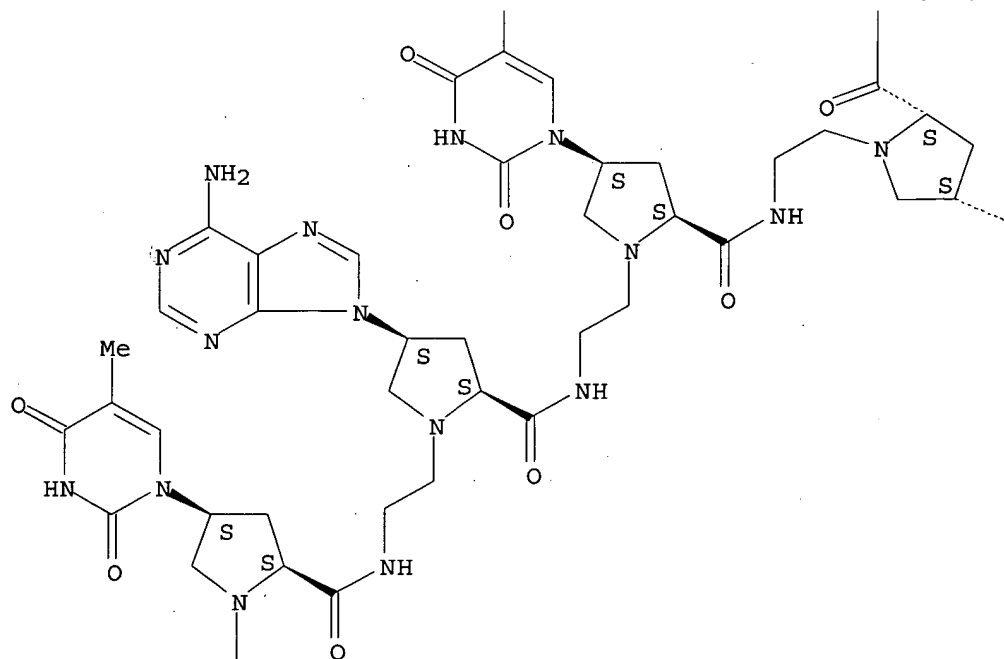
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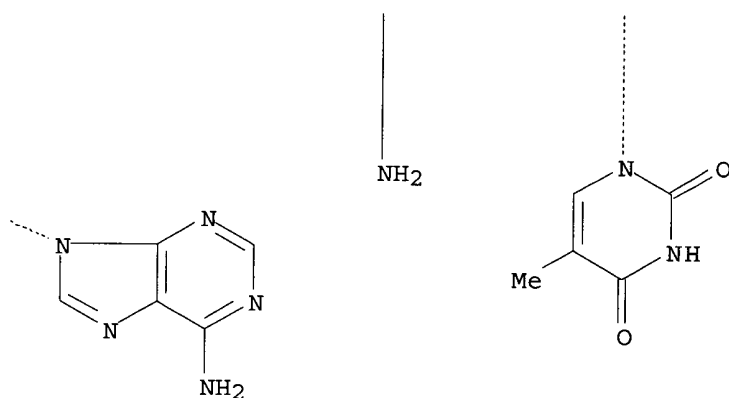
PAGE 1-B



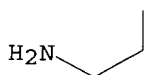
PAGE 2-A



PAGE 2-B



PAGE 3-A



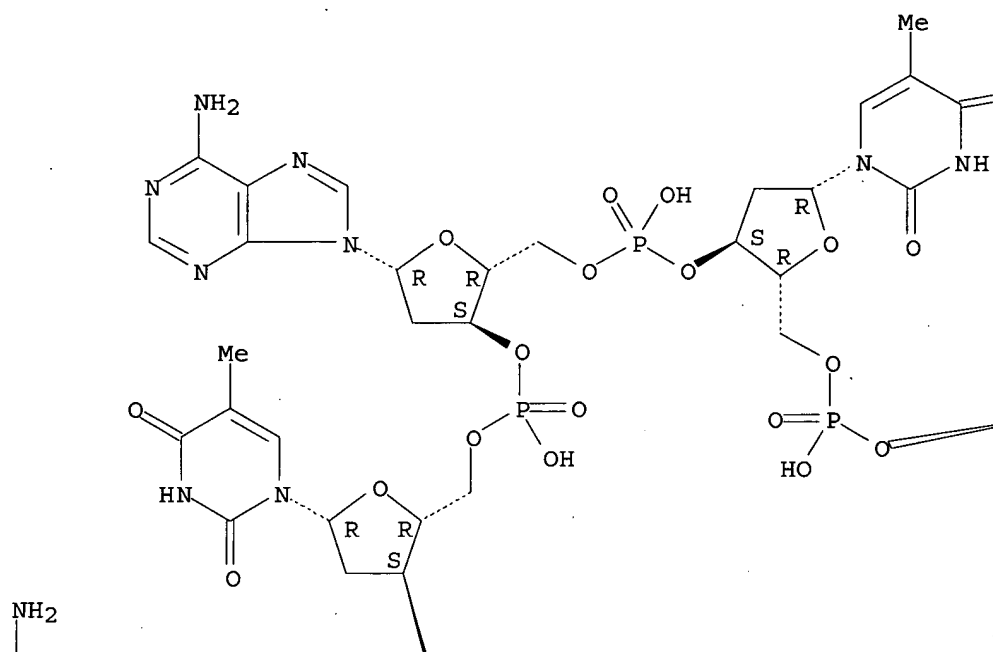
RN 386212-24-4 HCAPLUS
 CN Adenosine, 2'-deoxyadenylyl-(3'→5')-2'-deoxyadenylyl-(3'→5')-thymidylyl-(3'→5')-thymidylyl-(3'→5')-thymidylyl-(3'→5')-2'-deoxyadenylyl-(3'→5')-thymidylyl-(3'→5')-2'-deoxy-, complex with peptide nucleic acid (H-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-L-prolyl-(4S)-1-(2-aminoethyl)-4-(6-amino-9H-purin-9-yl)-L-prolyl-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-L-prolyl-(4S)-1-(2-aminoethyl)-4-(6-amino-9H-purin-9-yl)-L-prolyl-(4S)-1-(2-aminoethyl)-4-(6-amino-9H-purin-9-yl)-L-prolyl-(4S)-1-(2-aminoethyl)-4-(6-amino-9H-purin-9-yl)-L-prolyl-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-L-prolyl-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-L-prolyl)-Lys-NH₂ (1:1) (9CI) (CA INDEX NAME)

CM 1

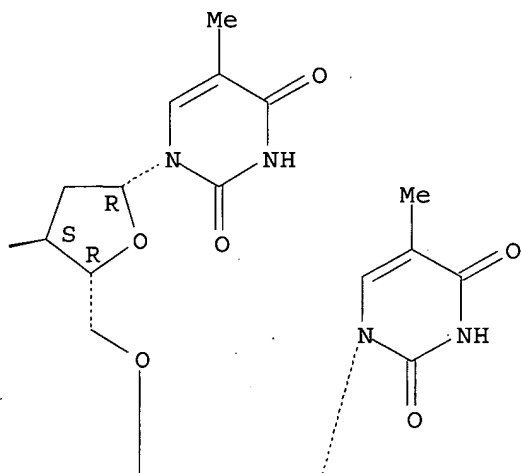
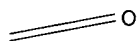
CRN 386212-23-3
 CMF C80 H101 N28 O46 P7

Absolute stereochemistry.

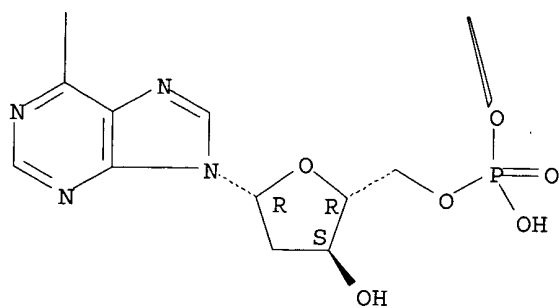
PAGE 1-A



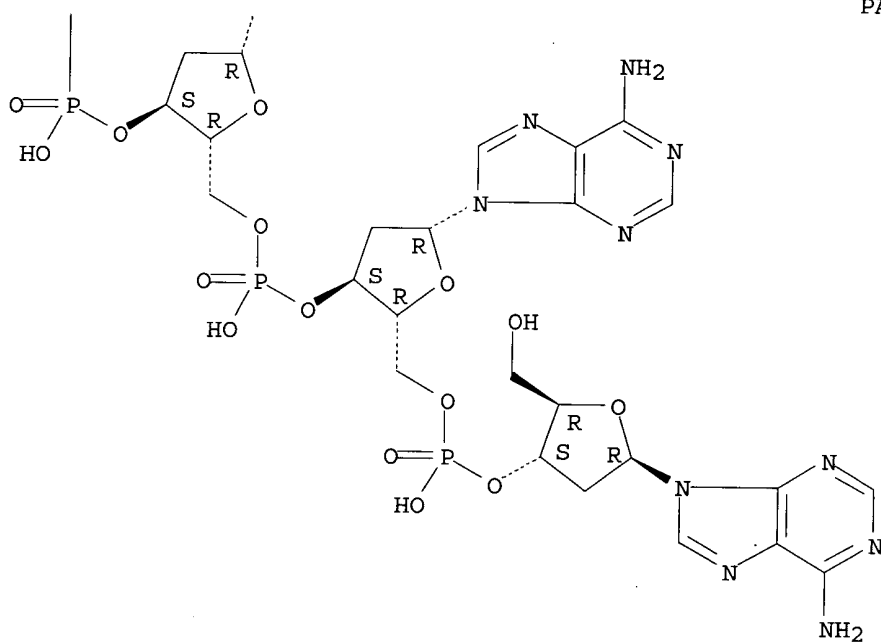
PAGE 1-B



PAGE 2-A



PAGE 2-B



CM 2

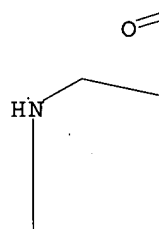
CRN 386212-19-7

CMF C102 H139 N47 O17

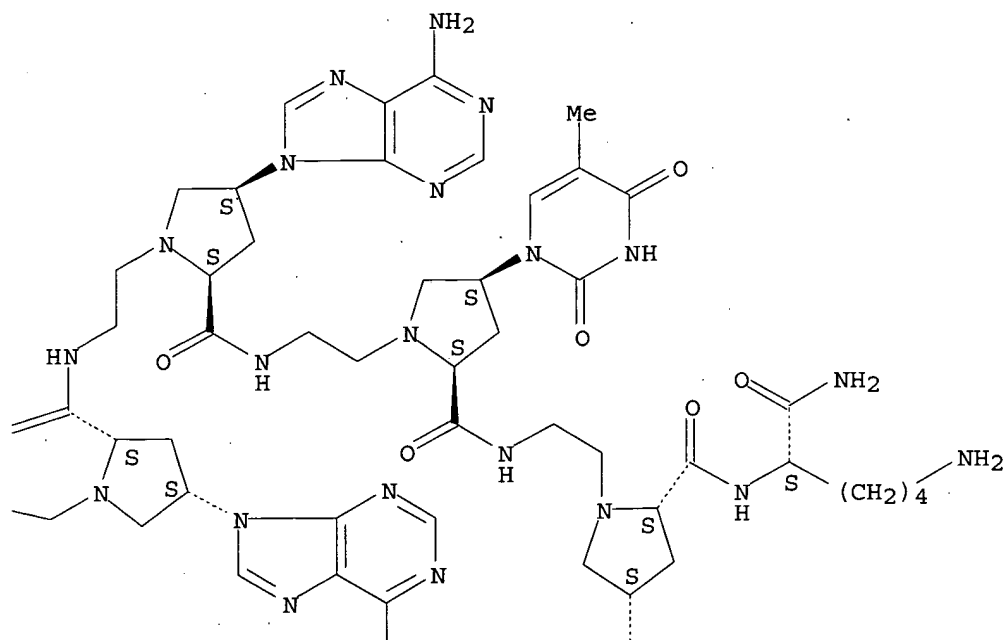
Absolute stereochemistry.

PAGE 1-A

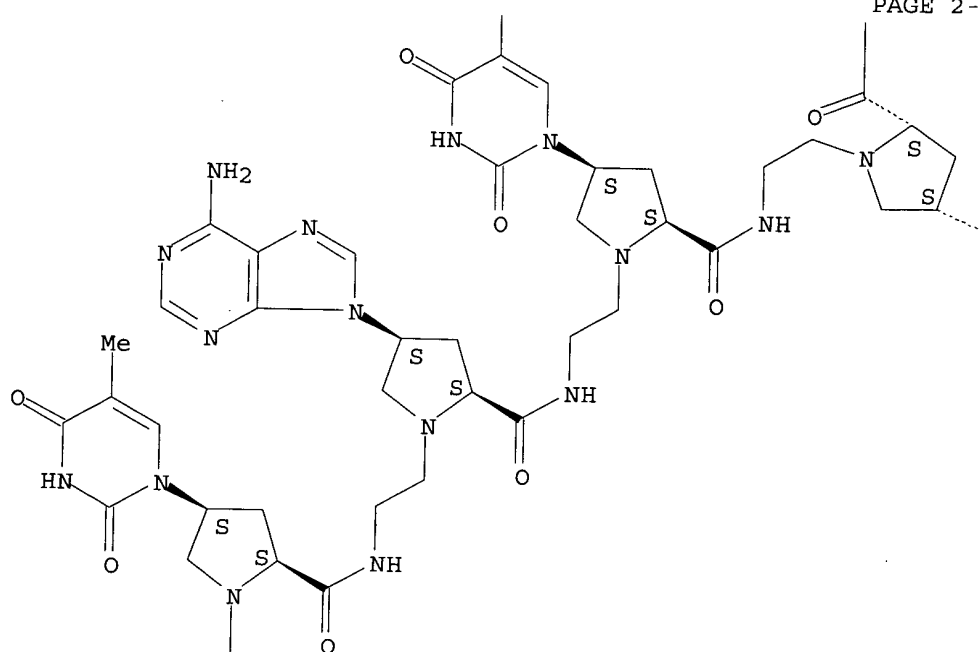
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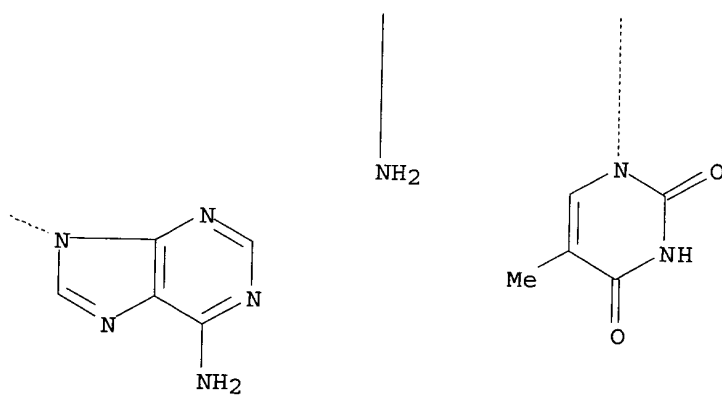
PAGE 1-B



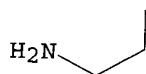
PAGE 2-A



PAGE 2-B



PAGE 3-A



IT 253307-71-0P 340961-43-5P 340961-45-7P
371970-41-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

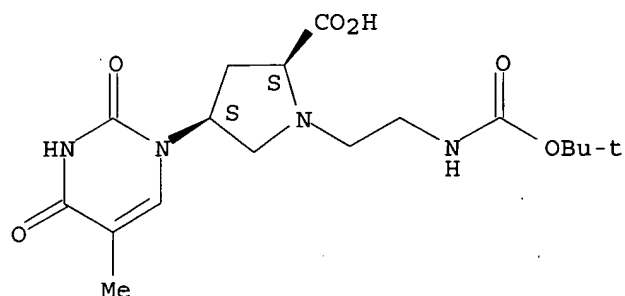
(preparation of cis-L-proline-based PNA oligomers and their hybridization)

characteristics with DNA)

RN 253307-71-0 HCAPLUS

CN L-Proline, 4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-1-[2-
[[1,1-dimethylethoxy)carbonyl]amino]ethyl]-, (4S)-(9CI) (CA INDEX NAME)

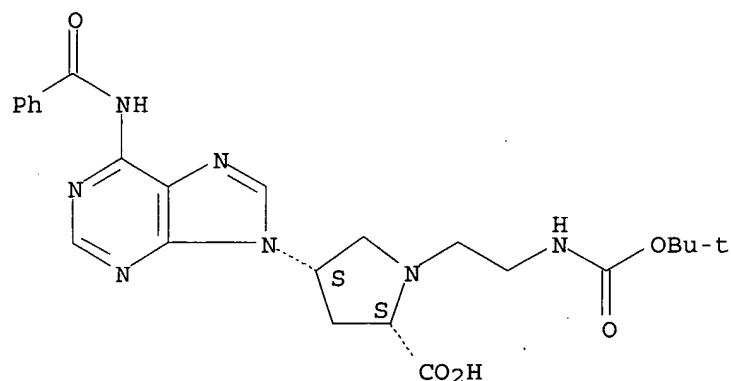
Absolute stereochemistry.



RN 340961-43-5 HCAPLUS

CN L-Proline, 4-[6-(benzoylamino)-9H-purin-9-yl]-1-[2-[[1,1-
dimethylethoxy)carbonyl]amino]ethyl]-, (4S)-(9CI) (CA INDEX NAME)

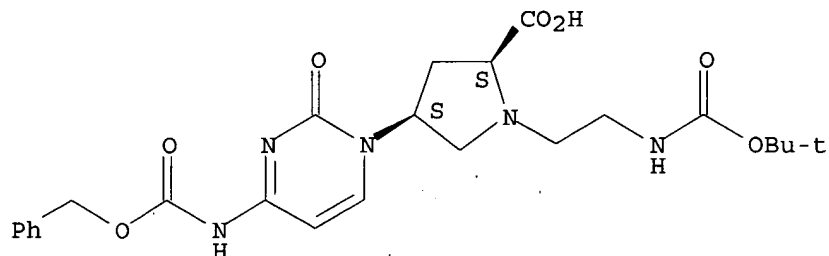
Absolute stereochemistry.



RN 340961-45-7 HCAPLUS

CN L-Proline, 1-[2-[[1,1-dimethylethoxy)carbonyl]amino]ethyl]-4-[2-oxo-4-
[[1,1-dimethylethoxy)carbonyl]amino]-1(2H)-pyrimidinyl]-, (4S)-(9CI) (CA
INDEX NAME)

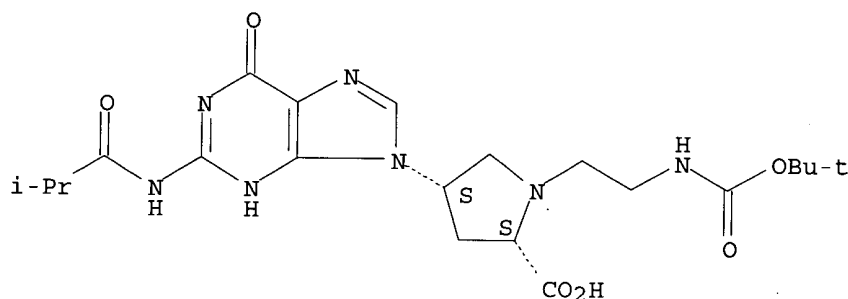
Absolute stereochemistry.



RN 371970-41-1 HCAPLUS

CN L-Proline, 4-[1,6-dihydro-2-[(2-methyl-1-oxopropyl)amino]-6-oxo-9H-purin-9-yl]-1-[2-[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 386212-19-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of cis-L-proline-based PNA oligomers and their hybridization characteristics with DNA)

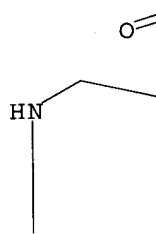
RN 386212-19-7 HCAPLUS

CN Peptide nucleic acid, (H-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-L-prolyl-(4S)-1-(2-aminoethyl)-4-(6-amino-9H-purin-9-yl)-L-prolyl-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-L-prolyl-(4S)-1-(2-aminoethyl)-4-(6-amino-9H-purin-9-yl)-L-prolyl-(4S)-1-(2-aminoethyl)-4-(6-amino-9H-purin-9-yl)-L-prolyl-(4S)-1-(2-aminoethyl)-4-(6-amino-9H-purin-9-yl)-L-prolyl-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-L-prolyl-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-L-prolyl)-Lys-NH2 (9CI) (CA INDEX NAME)

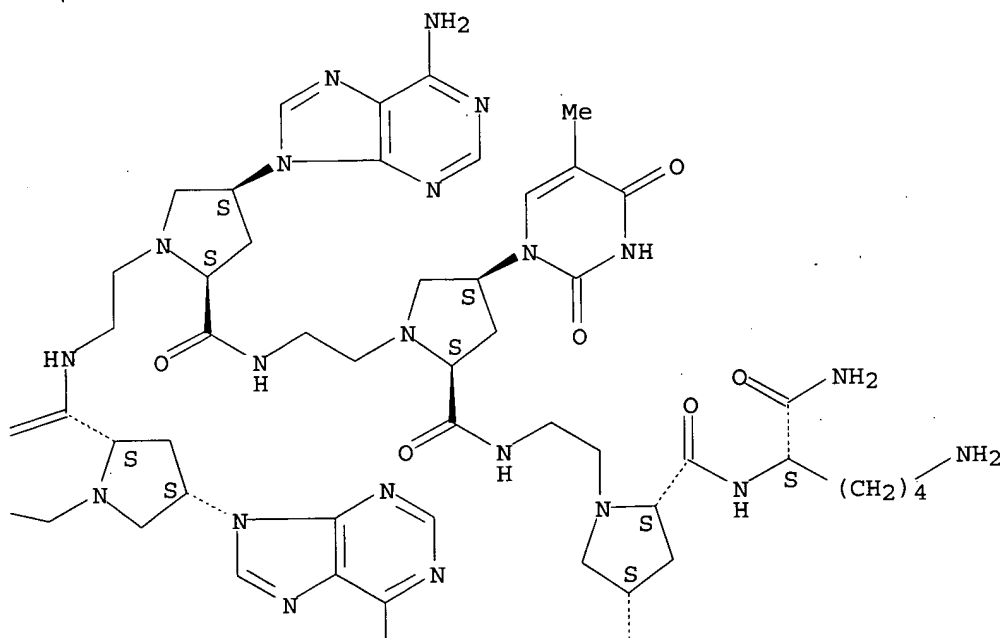
Absolute stereochemistry.

PAGE 1-A

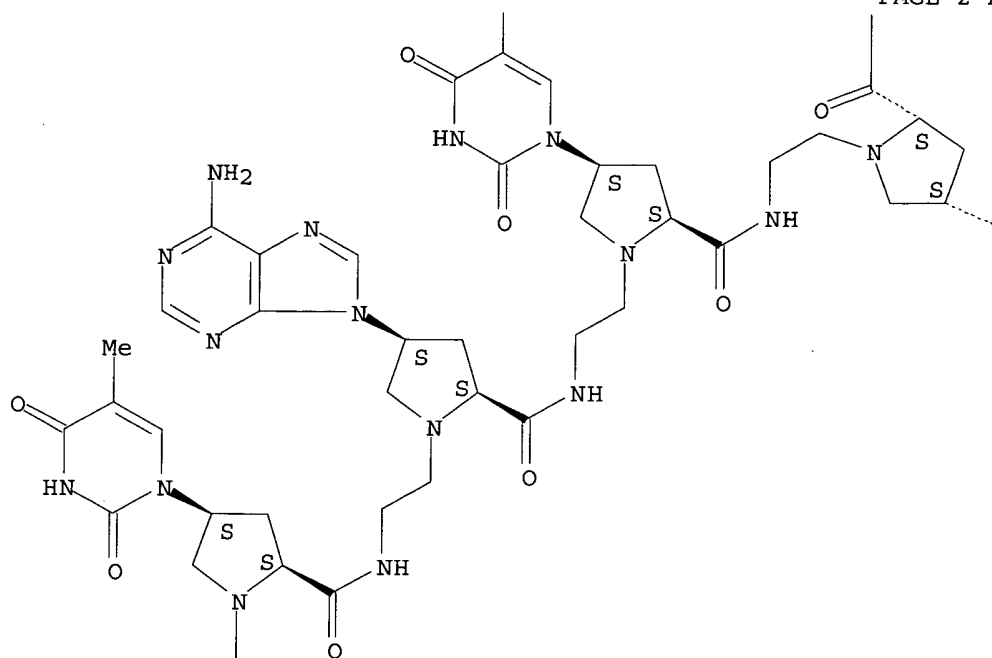
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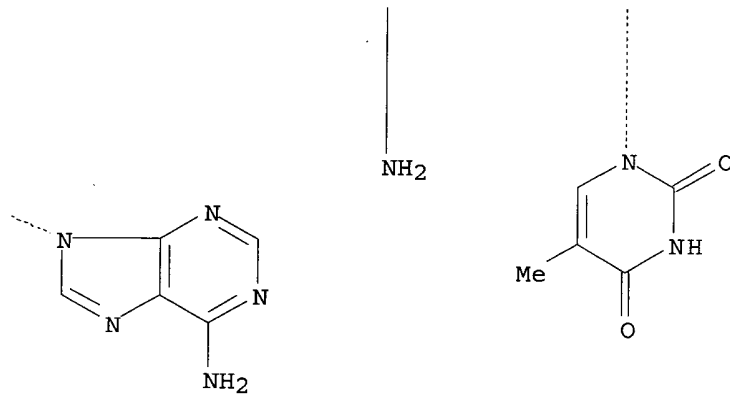
PAGE 1-B



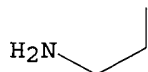
PAGE 2-A



PAGE 2-B



PAGE 3-A



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L38 ANSWER 8 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 2001:675176 HCAPLUS

DOCUMENT NUMBER: 135:354283
 TITLE: Engineering preferences of hairpin PNA binding to complementary DNA: effect of N7G in aeg/aep PNA backbone
 AUTHOR(S): Kumar, V. A.; D'Costa, M.; Ganesh, K. N.
 CORPORATE SOURCE: Division of Organic Chemistry (Synthesis), National Chemical Laboratory, Pune, India
 SOURCE: Nucleosides, Nucleotides & Nucleic Acids (2001), 20(4-7), 1187-1191
 CODEN: NNNAFY; ISSN: 1525-7770
 PUBLISHER: Marcel Dekker, Inc.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 135:354283

AB Aminoethylglycyl peptide nucleic acid (aegPNA) and aminoethylpropyl peptide nucleic acid (aepPNA) monomeric units bearing the N7-guanine nucleobase as a substitute for protonated cytosine (C+) have been shown to bind to a GC base-pair of a duplex in a pH-independent manner when placed in the third strand. The aepPNA backbone exerts a preference for binding in the antiparallel Hoogsteen mode over the parallel Hoogsteen mode.

CC 6-2 (General Biochemistry)

IT 289684-58-8P 340961-45-7P 371970-41-1P
 RL: PNU (Preparation, unclassified); PREP (Preparation)
 (recognition of DNA is influenced by presence of aminoethylpropyl peptide nucleic acid units in triplex-forming PNA hairpins)

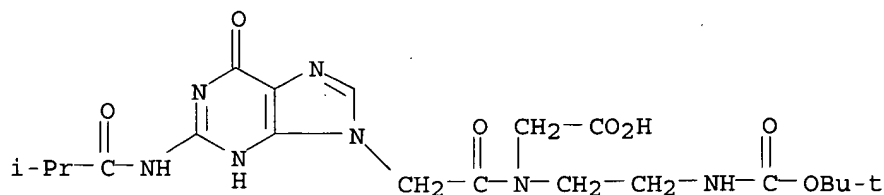
IT 340961-32-2P 340961-34-4P 371970-39-7P
 371970-40-0P
 RL: PNU (Preparation, unclassified); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
 (recognition of DNA is influenced by presence of aminoethylpropyl peptide nucleic acid units in triplex-forming PNA hairpins)

IT 21047-89-2, N2-Isobutyrylguanine 149411-91-6 169566-58-9
 253307-68-5
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (recognition of DNA is influenced by presence of aminoethylpropyl peptide nucleic acid units in triplex-forming PNA hairpins)

IT 289684-58-8P 340961-45-7P 371970-41-1P
 RL: PNU (Preparation, unclassified); PREP (Preparation)
 (recognition of DNA is influenced by presence of aminoethylpropyl peptide nucleic acid units in triplex-forming PNA hairpins)

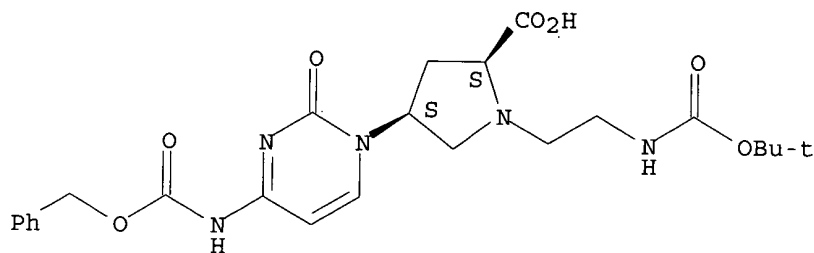
RN 289684-58-8 HCAPLUS

CN Glycine, N-[[[1,6-dihydro-2-[(2-methyl-1-oxopropyl)amino]-6-oxo-9H-purin-9-yl]acetyl]-N-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]- (9CI) (CA INDEX NAME)



RN 340961-45-7 HCAPLUS
 CN L-Proline, 1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-4-[2-oxo-4-[[[(phenylmethoxy)carbonyl]amino]-1(2H)-pyrimidinyl]-, (4S)- (9CI) (CA INDEX NAME)

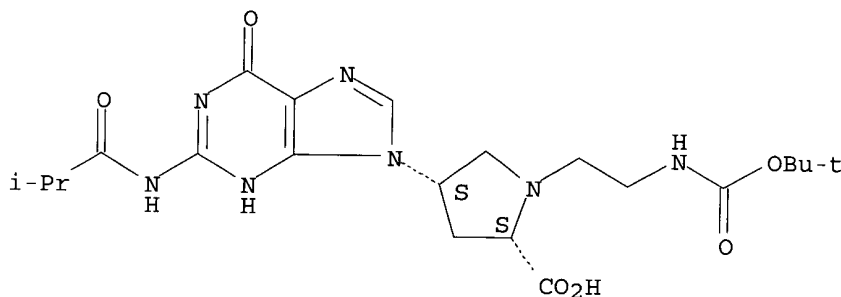
Absolute stereochemistry.



RN 371970-41-1 HCAPLUS

CN L-Proline, 4-[1,6-dihydro-2-[(2-methyl-1-oxopropyl)amino]-6-oxo-9H-purin-9-yl]-1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



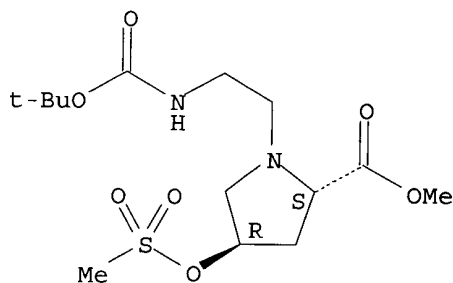
IT 340961-32-2P 340961-34-4P 371970-39-7P
371970-40-0P

RL: PNU (Preparation, unclassified); RCT (Reactant); PREP (Preparation);
RACT (Reactant or reagent)
(recognition of DNA is influenced by presence of aminoethylpropyl
peptide nucleic acid units in triplex-forming PNA hairpins)

RN 340961-32-2 HCAPLUS

CN L-Proline, 1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-4-
[(methylsulfonyl)oxy]-, methyl ester, (4R)- (9CI) (CA INDEX NAME)

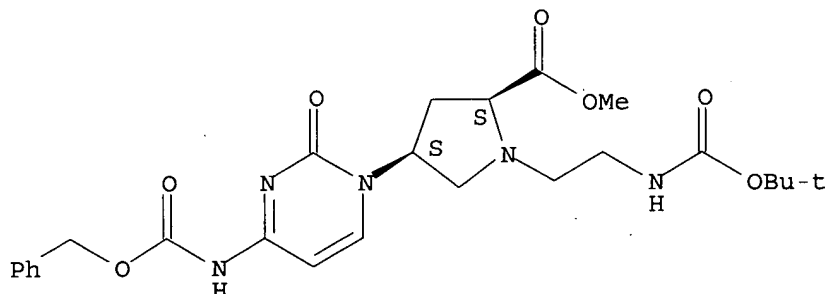
Absolute stereochemistry.



RN 340961-34-4 HCAPLUS

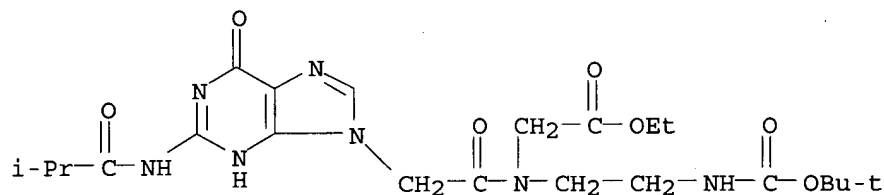
CN L-Proline, 1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-4-[2-oxo-4-[[[phenylmethoxy)carbonyl]amino]-1(2H)-pyrimidinyl]-, methyl ester, (4S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 371970-39-7 HCAPLUS

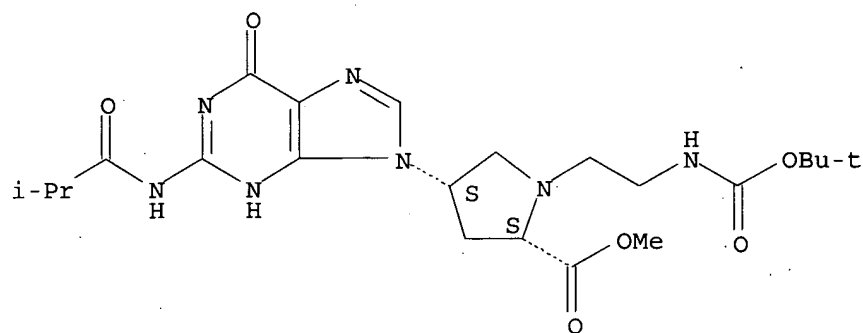
CN Glycine, N-[[[1,6-dihydro-2-[(2-methyl-1-oxopropyl)amino]-6-oxo-9H-purin-9-yl]acetyl]-N-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 371970-40-0 HCAPLUS

CN L-Proline, 4-[1,6-dihydro-2-[(2-methyl-1-oxopropyl)amino]-6-oxo-9H-purin-9-yl]-1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, methyl ester, (4S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



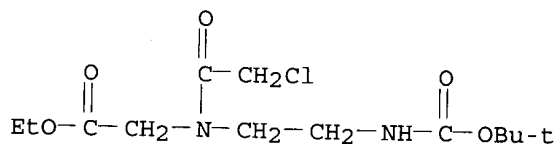
IT 169566-58-9 253307-68-5

RL: RCT (Reactant); RACT (Reactant or reagent)

(recognition of DNA is influenced by presence of aminoethylpropyl peptide nucleic acid units in triplex-forming PNA hairpins)

RN 169566-58-9 HCAPLUS

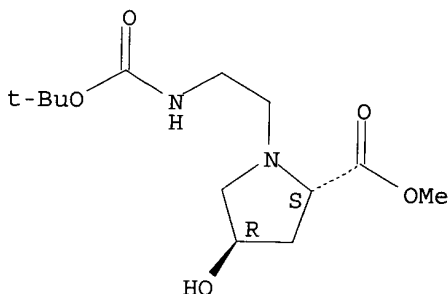
CN Glycine, N-(chloroacetyl)-N-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-ethyl ester (9CI) (CA INDEX NAME)



RN 253307-68-5 HCAPLUS

CN L-Proline, 1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-4-hydroxy-, methyl ester, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

6

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L38 ANSWER 9 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:259380 HCAPLUS

DOCUMENT NUMBER: 135:107316

TITLE: The synthesis of L-proline derived hexaazamacrocyclic ligands of C3 symmetry via intramolecular methyl ester aminolysis

AUTHOR(S): Achmatowicz, M.; Jurczak, J.

CORPORATE SOURCE: Institute of Organic Chemistry, Polish Academy of Sciences, Warsaw, PL-01-224, Pol.

SOURCE: Tetrahedron: Asymmetry (2001), 12(3), 487-495

CODEN: TASYE3; ISSN: 0957-4166

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:107316

AB A convenient synthesis of enantiomerically pure 18-, 21-, and 24-membered hexaaza-crown ligands is presented. Linear α,ω -aminoesters, prepared from L-proline, undergo intramol. aminolysis to afford the corresponding 18-, 21-, and 24-membered macrocyclic amides in satisfactory yields (42, 65, and 22%, resp.). These were subsequently transformed into the title macrocyclic hexamines via exhaustive reduction with a borane-dimethyl sulfide complex. X-ray structures of two larger macrocyclic amides are also presented.

CC 28-23 (Heterocyclic Compounds (More Than One Hetero Atom))

IT 295343-27-0 295343-33-8 343248-65-7 343248-67-9

350028-08-9 350028-09-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of L-proline derived hexaazamacrocyclic ligands of C3 symmetry via intramol. Me ester aminolysis)

IT 343248-65-7 350028-08-9

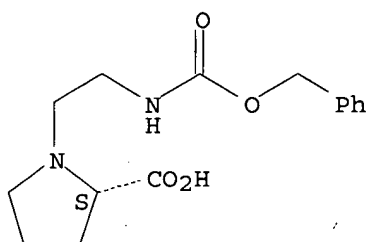
RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of L-proline derived hexaazamacrocyclic ligands of C3 symmetry via intramol. Me ester aminolysis)

RN 343248-65-7 HCAPLUS

CN L-Proline, 1-[2-[[[(phenylmethoxy) carbonyl] amino] ethyl] - (9CI) (CA INDEX NAME)

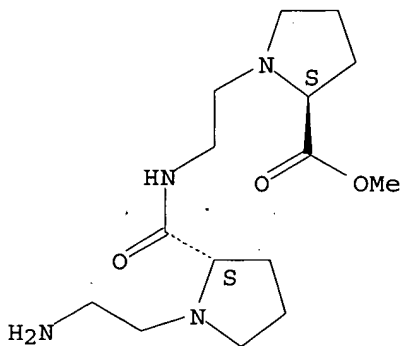
Absolute stereochemistry.



RN 350028-08-9 HCAPLUS

CN L-Proline, 1-[2-[[[(2S)-1-(2-aminoethyl)-2-pyrrolidinyl] carbonyl] amino] ethyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L38 ANSWER 10 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:663052 HCAPLUS

DOCUMENT NUMBER: 132:251401

TITLE: Aminoethylprolyl Peptide Nucleic Acids (aepPNA):
Chiral PNA Analogues That Form Highly Stable
DNA:aepPNA2 Triplexes

AUTHOR(S): D'Costa, Moneesha; Kumar, Vaijayanti A.; Ganesh,
Krishna N.

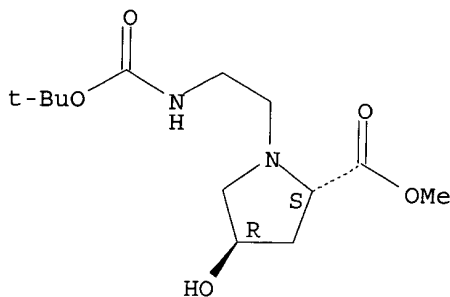
CORPORATE SOURCE: Division of Organic Chemistry (Synthesis), National
Chemical Laboratory, Pune, 411008, India

SOURCE: Organic Letters (1999), 1(10), 1513-1516

PUBLISHER: CODEN: ORLEF7; ISSN: 1523-7060
 DOCUMENT TYPE: American Chemical Society
 LANGUAGE: English

- AB The replacement of the glycyl component in the peptide nucleic acid (PNA) backbone by a prolyl unit bearing a nucleobase leads to the aminoethylprolyl (aep) PNAs, which are chiral and cationic. The homo-oligomeric aepPNA binds to complementary DNA sequences with high affinity and sequence specificity, forming highly stable triplexes.
- CC 34-3 (Amino Acids, Peptides, and Proteins)
 Section cross-reference(s): 33
- IT 40216-83-9P 114676-59-4P 253307-68-5P 253307-69-6P
 253307-71-0P 253307-73-2P 253307-74-3P
 253307-76-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and reaction of in the synthesis of aminoethylprolyl peptide nucleic acids)
- IT 262614-79-9P 262614-81-3P 262615-03-2P
 262615-29-2P 262615-33-8P 262615-36-1P
 262615-38-3P 262615-58-7P 262615-78-1P
 262615-79-2P 262615-84-9P 262615-88-3P
 262615-89-4P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (preparation and triplex stability of)
- IT 253307-78-7P 253307-80-1P 253307-82-3P
 253307-84-5P 253342-10-8P 253342-11-9P
 253342-12-0P 253342-13-1P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (preparation and triplex-forming properties of as chiral PNA analogs)
- IT 253307-86-7P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (preparation and triplex-forming properties of as comparison for chiral PNA analogs)
- IT 253307-68-5P 253307-69-6P 253307-71-0P
 253307-73-2P 253307-74-3P 253307-76-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and reaction of in the synthesis of aminoethylprolyl peptide nucleic acids)
- RN 253307-68-5 HCAPLUS
- CN L-Proline, 1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-4-hydroxy-, methyl ester, (4R)-(9CI) (CA INDEX NAME)

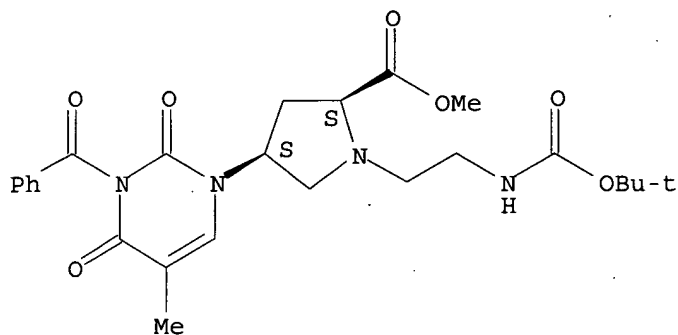
Absolute stereochemistry.



RN 253307-69-6 HCAPLUS

CN L-Proline, 4-(3-benzoyl-3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-
1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, methyl ester, (4S)-
(9CI) (CA INDEX NAME)

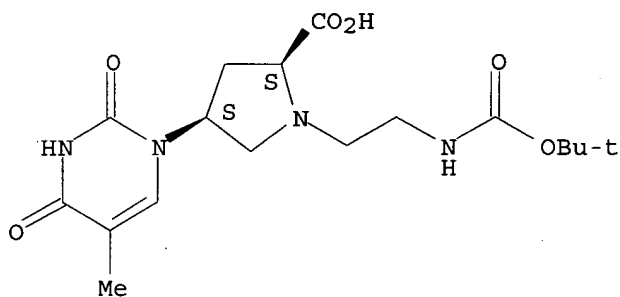
Absolute stereochemistry.



RN 253307-71-0 HCAPLUS

CN L-Proline, 4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-1-[2-
[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, (4S)- (9CI) (CA INDEX NAME)

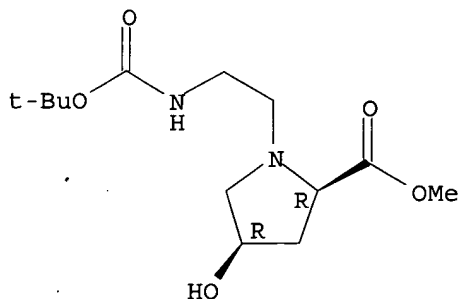
Absolute stereochemistry.



RN 253307-73-2 HCAPLUS

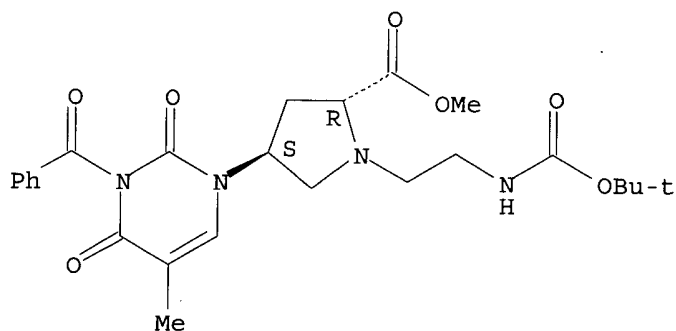
CN D-Proline, 1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-4-hydroxy-,
methyl ester, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



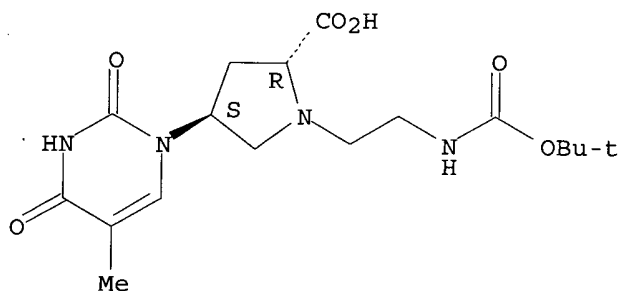
RN 253307-74-3 HCAPLUS
 CN D-Proline, 4-(3-benzoyl-3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, methyl ester, (4S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 253307-76-5 HCAPLUS
 CN D-Proline, 4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, (4S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 262614-79-9P 262614-81-3P 262615-03-2P
 262615-29-2P 262615-33-8P 262615-36-1P
 262615-38-3P 262615-58-7P 262615-78-1P
 262615-79-2P 262615-84-9P 262615-88-3P
 262615-89-4P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (preparation and triplex stability of)

RN 262614-79-9 HCAPLUS

CN DNA, d(G-C-A-A-A-A-A-A-A-C-G), complex with peptide nucleic acid
 (H-T-T-T-T-T-T-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro)-Bal-OH (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 262408-13-9

CMF Unspecified

CCI MAN

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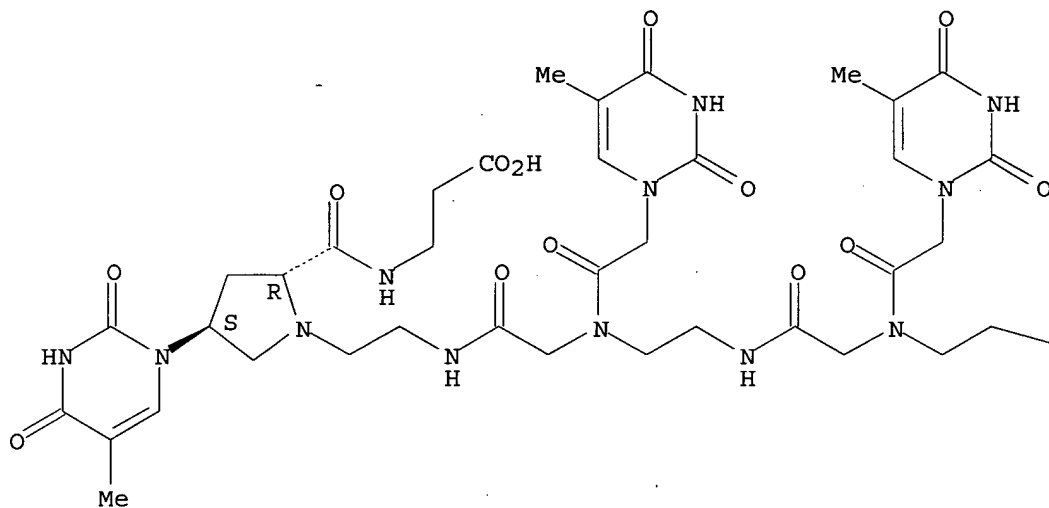
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CRN 253307-78-7

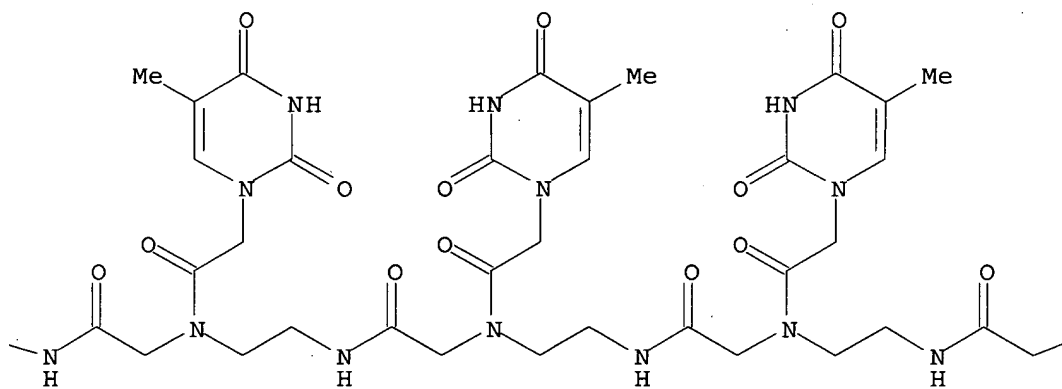
CMF C92 H121 N33 O33

Absolute stereochemistry.

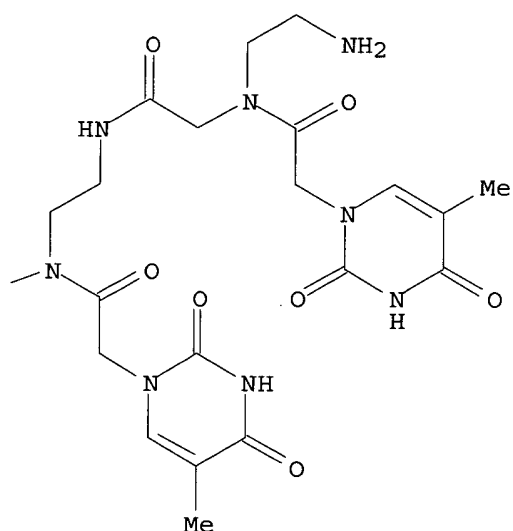
PAGE 1-A



PAGE 1-B



PAGE 1-C



RN 262614-81-3 HCAPLUS
CN DNA, d(G-C-A-A-A-A-A-A-A-C-G), complex with peptide nucleic acid
(H-T-T-T-T-T-T-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-
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CRN 262408-13-9
CMF Unspecified
CCI MAN

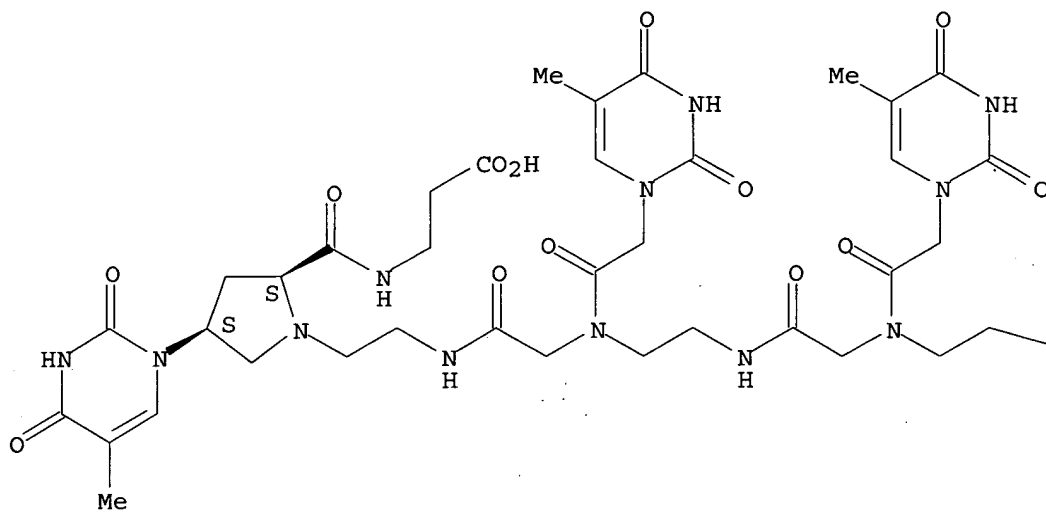
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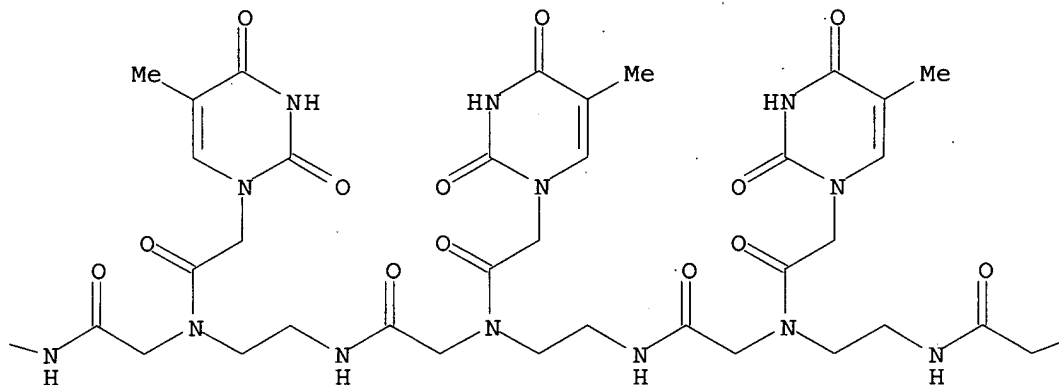
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CMF C92 H121 N33 O33

Absolute stereochemistry.

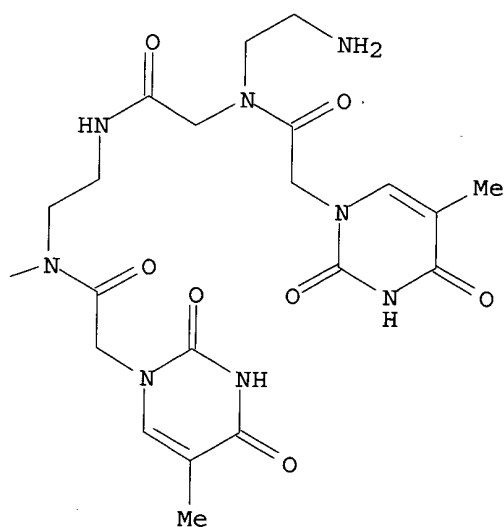
PAGE 1-A



PAGE 1-B



PAGE 1-C



RN 262615-03-2 HCAPLUS
 CN DNA, d(G-C-A-A-A-A-A-A-A-A-C-G), complex with peptide nucleic acid
 (H-T-T-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-
 pyrimidinyl)-D-Pro-T-T-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-
 dioxo-1(2H)-pyrimidinyl)-D-Pro)-Bal-OH (1:2) (9CI) (CA INDEX NAME)

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CRN 262408-13-9
 CMF Unspecified
 CCI MAN

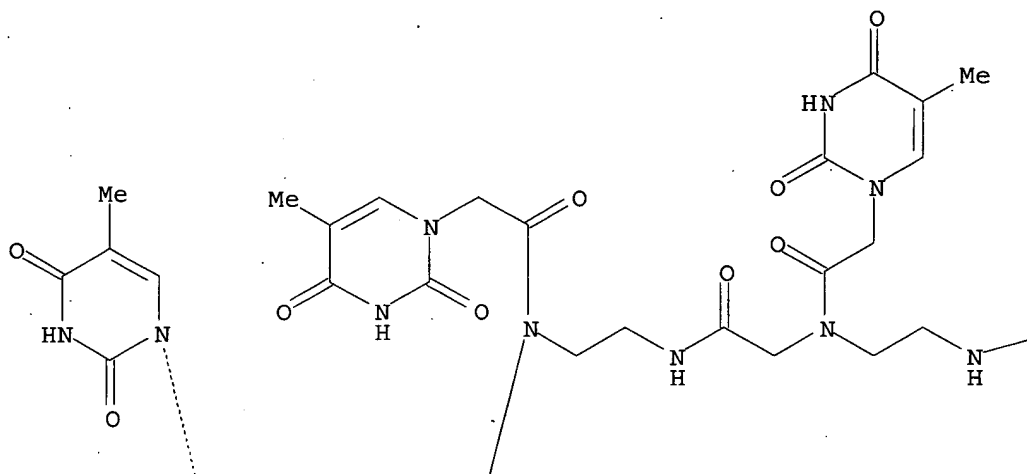
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CM 2

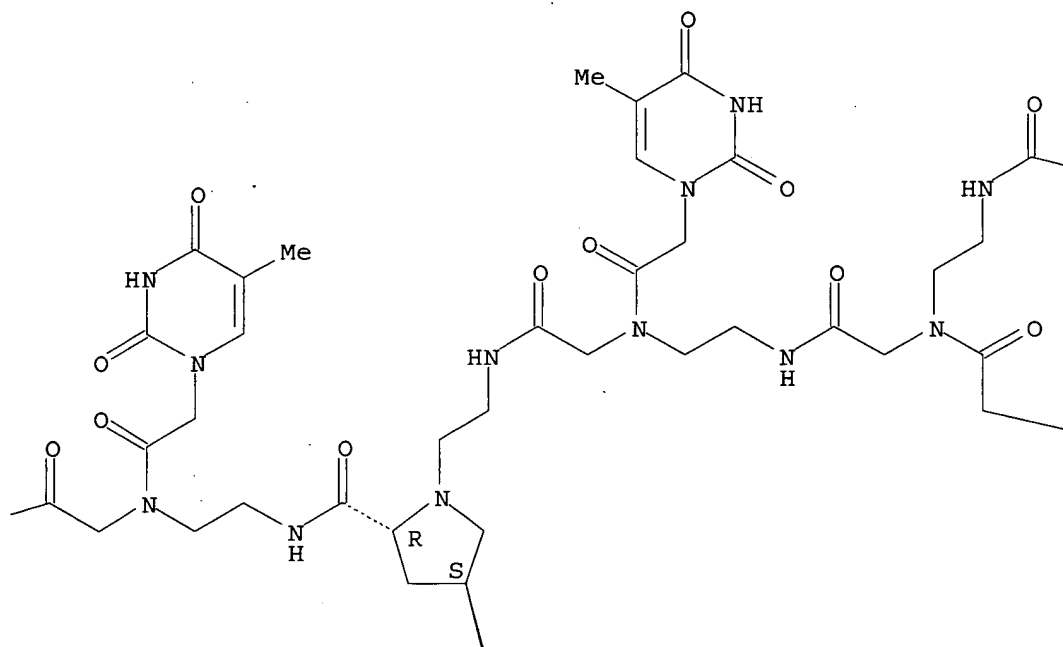
CRN 253307-82-3
 CMF C93 H123 N33 O32

Absolute stereochemistry.

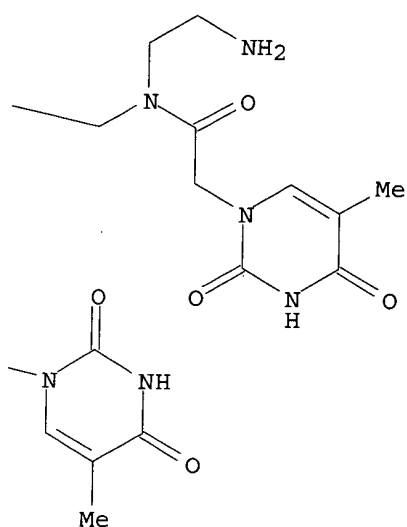
PAGE 1-A



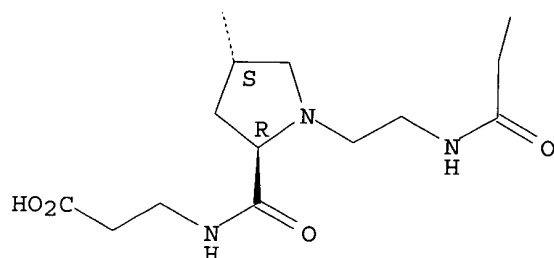
PAGE 1-B



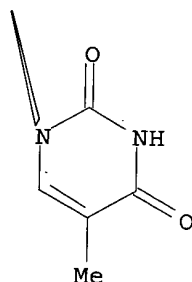
PAGE 1-C



PAGE 2-A



PAGE 2-B



RN 262615-29-2 HCAPLUS
 CN DNA, d(G-C-A-A-A-A-A-A-C-G), complex with peptide nucleic acid
 (H-T-T-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-
 pyrimidinyl)-Pro-T-T-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-
 dioxo-1(2H)-pyrimidinyl)-Pro)-Bal-OH (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 262408-13-9

CMF Unspecified

CCI MAN

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

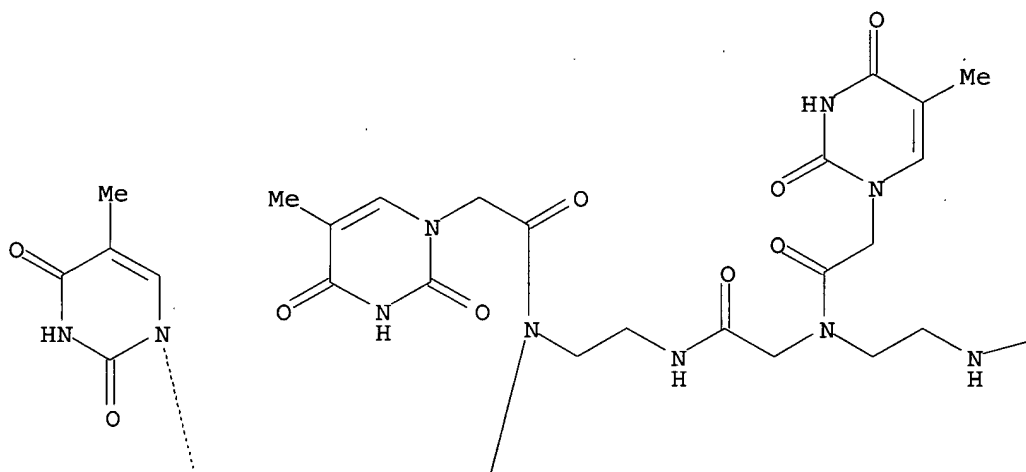
CM 2

CRN 253307-84-5

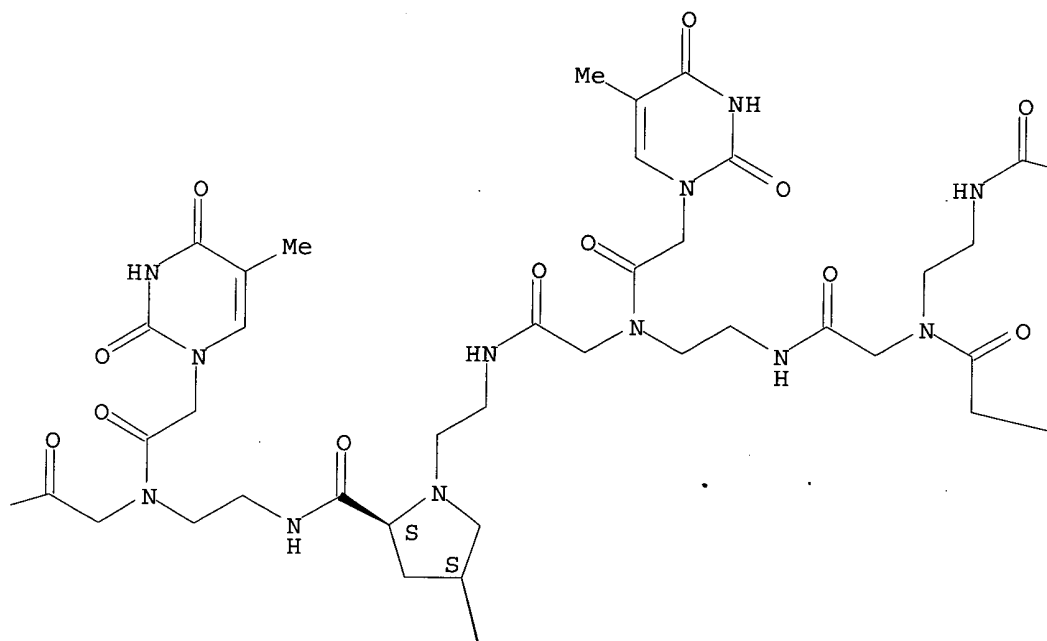
CMF C93 H123 N33 O32

Absolute stereochemistry.

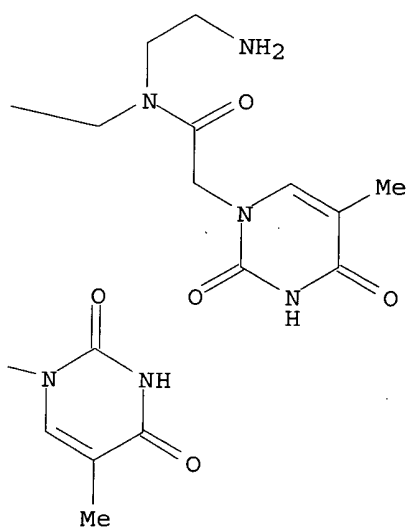
PAGE 1-A



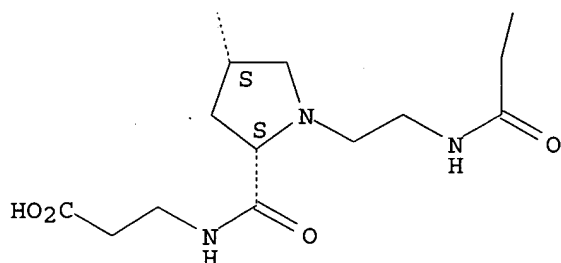
PAGE 1-B



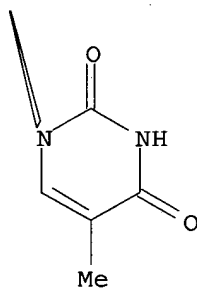
PAGE 1-C



PAGE 2-A



PAGE 2-B



RN 262615-33-8 HCAPLUS
 CN DNA, d(G-C-A-A-A-A-A-A-A-A-C-G), complex with peptide nucleic acid
 (H-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-
 pyrimidinyl)-D-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-
 dioxo-1(2H)-pyrimidinyl)-D-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-
 methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-
 dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro)-Bal-OH (1:2) (9CI)
 (CA INDEX NAME)

CM 1

CRN 262408-13-9

CMF Unspecified

CCI MAN

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

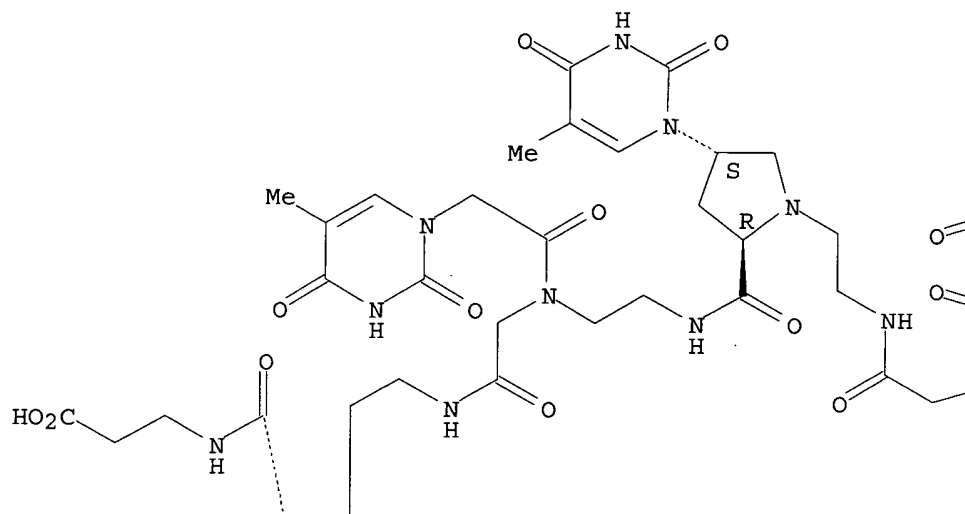
CM 2

CRN 253342-10-8

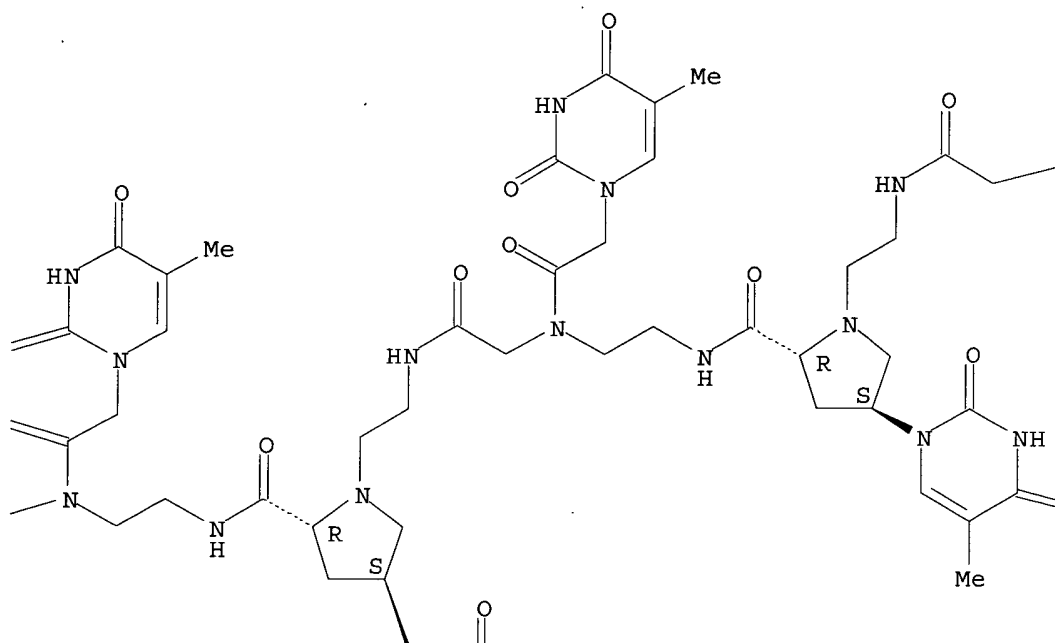
CMF C95 H127 N33 O30

Absolute stereochemistry.

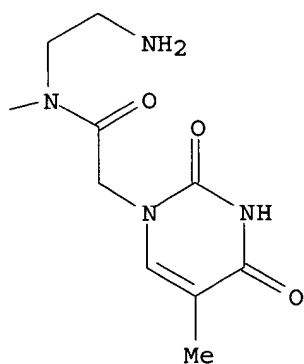
PAGE 1-A



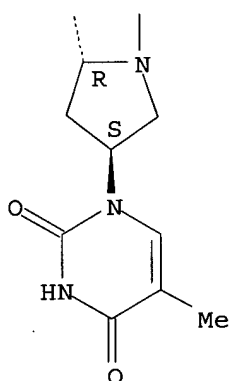
PAGE 1-B



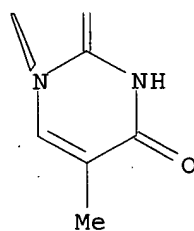
PAGE 1-C



PAGE 2-A



PAGE 2-B



RN 262615-36-1 HCAPLUS
 CN DNA, d(G-C-A-A-A-A-A-A-A-A-C-G), complex with peptide nucleic acid
 (H-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-
 pyrimidinyl)-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-
 1(2H)-pyrimidinyl)-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-

dioxo-1(2H)-pyrimidinyl)-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pro)-Bal-OH (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 262408-13-9

CMF Unspecified

CCI MAN

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

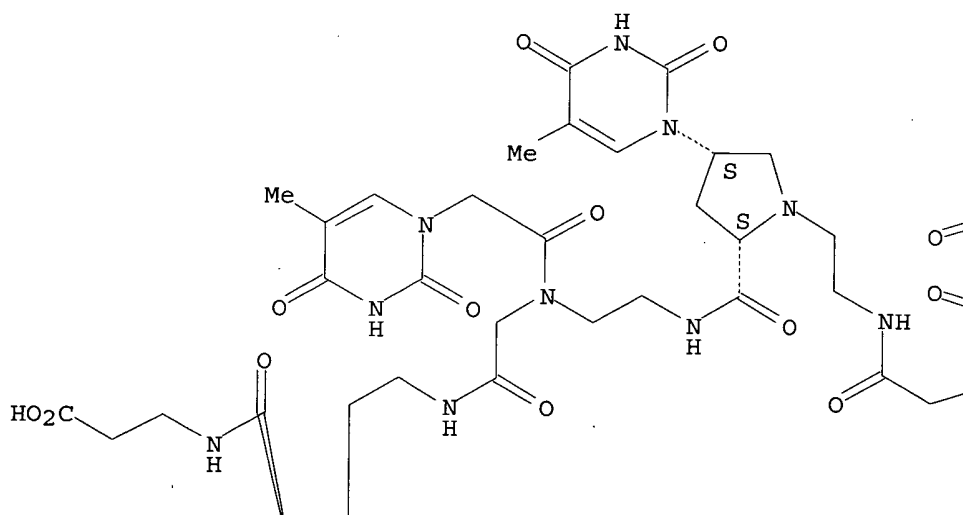
CM 2

CRN 253342-11-9

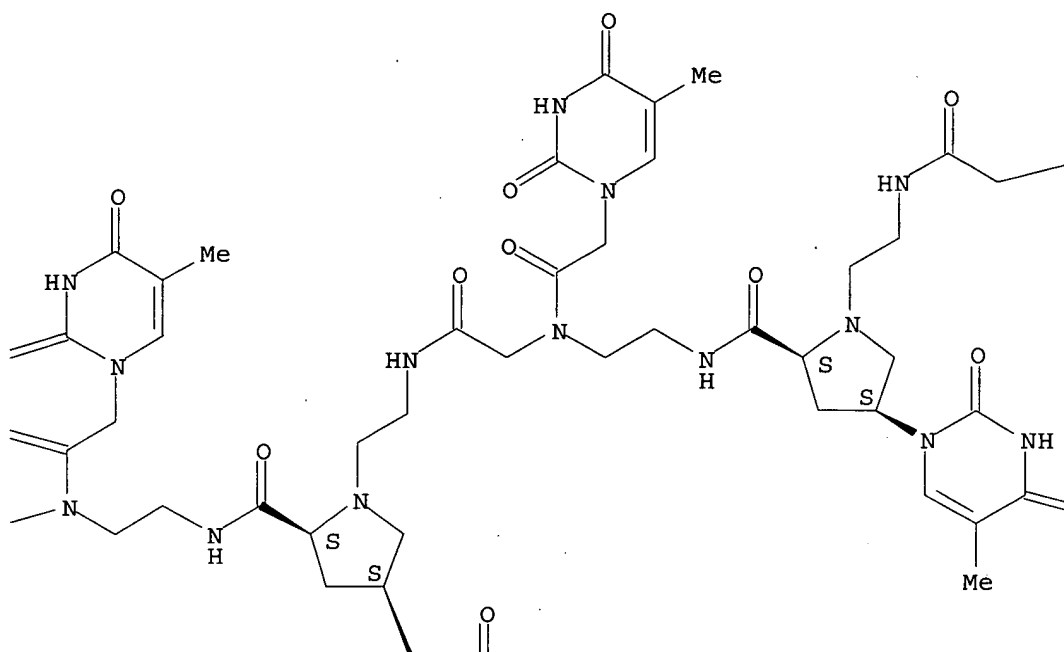
CMF C95 H127 N33 O30

Absolute stereochemistry.

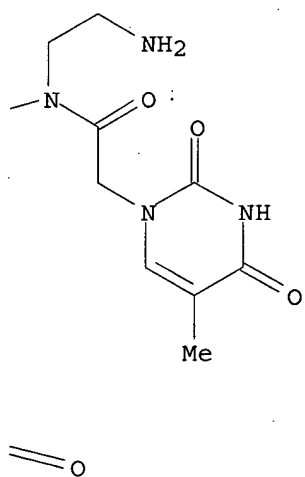
PAGE 1-A



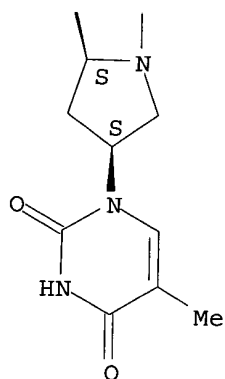
PAGE 1-B



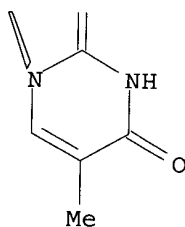
PAGE 1-C



PAGE 2-A



PAGE 2-B



RN 262615-38-3 HCAPLUS
 CN DNA, d(G-C-A-A-A-A-A-A-C-G), complex with peptide nucleic acid
 (H-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-
 pyrimidinyl)-D-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-
 1(2H)-pyrimidinyl)-D-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-
 dioxo-1(2H)-pyrimidinyl)-D-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-
 methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-
 dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-(4S)-1-(2-aminoethyl)-
 4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-(4S)-1-(2-
 aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-
 (4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-
 D-Pro)-Bal-OH (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 262408-13-9

CMF Unspecified

CCI MAN

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

CM 2

CRN 253342-12-0

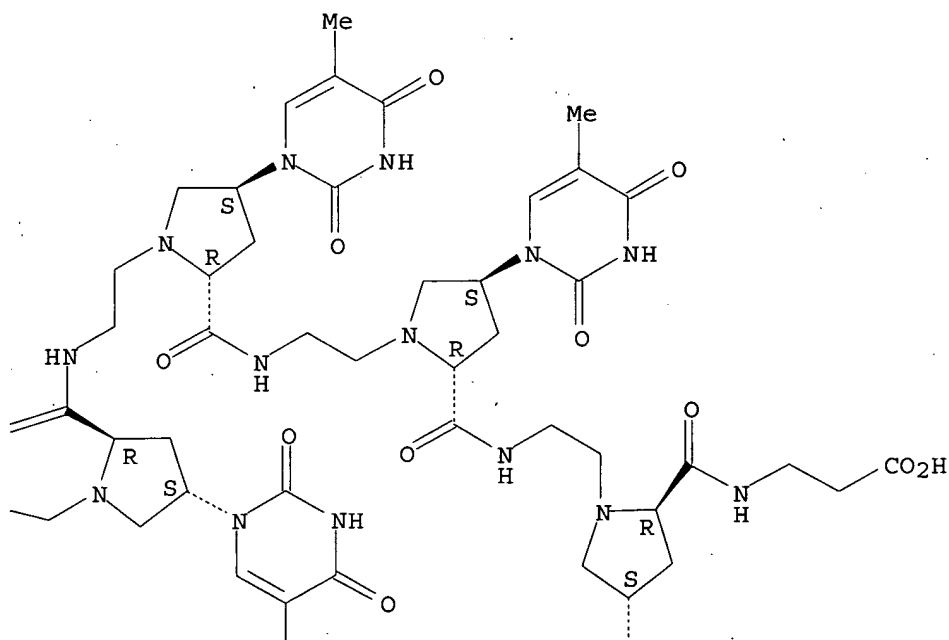
CMF C99 H135 N33 O26

Absolute stereochemistry.

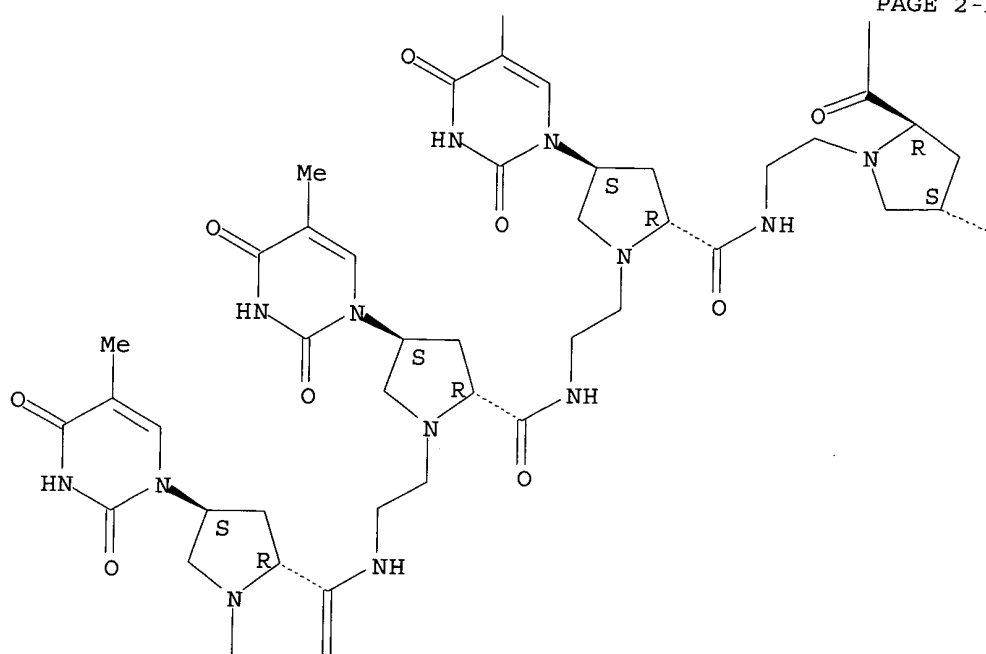
PAGE 1-A



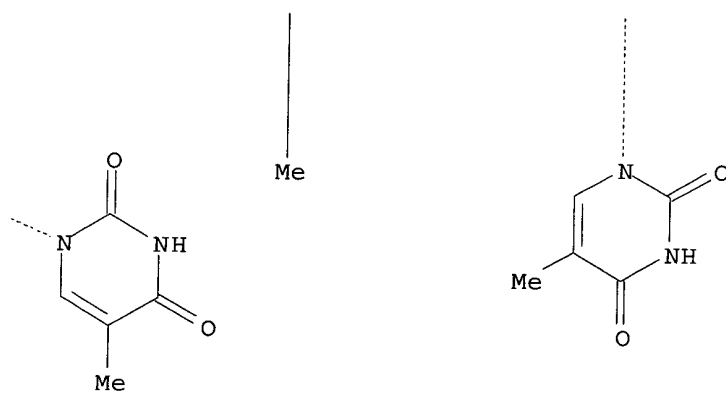
PAGE 1-B



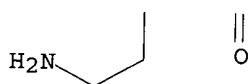
PAGE 2-A



PAGE 2-B



PAGE 3-A



RN 262615-58-7 HCAPLUS
 CN DNA, d(G-C-A-A-A-A-A-A-A-A-C-G), complex with peptide nucleic acid
 (H- (4S) -1- (2-aminoethyl) -4- (3,4-dihydro-5-methyl-2,4-dioxo-1(2H) -
 pyrimidinyl) -Pro- (4S) -1- (2-aminoethyl) -4- (3,4-dihydro-5-methyl-2,4-dioxo-
 1(2H) -pyrimidinyl) -Pro- (4S) -1- (2-aminoethyl) -4- (3,4-dihydro-5-methyl-2,4-

dioxo-1(2H)-pyrimidinyl)-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pro)-Bal-OH (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 262408-13-9

CMF Unspecified

CCI MAN

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

CM 2

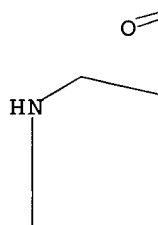
CRN 253342-13-1

CMF C99 H135 N33 O26

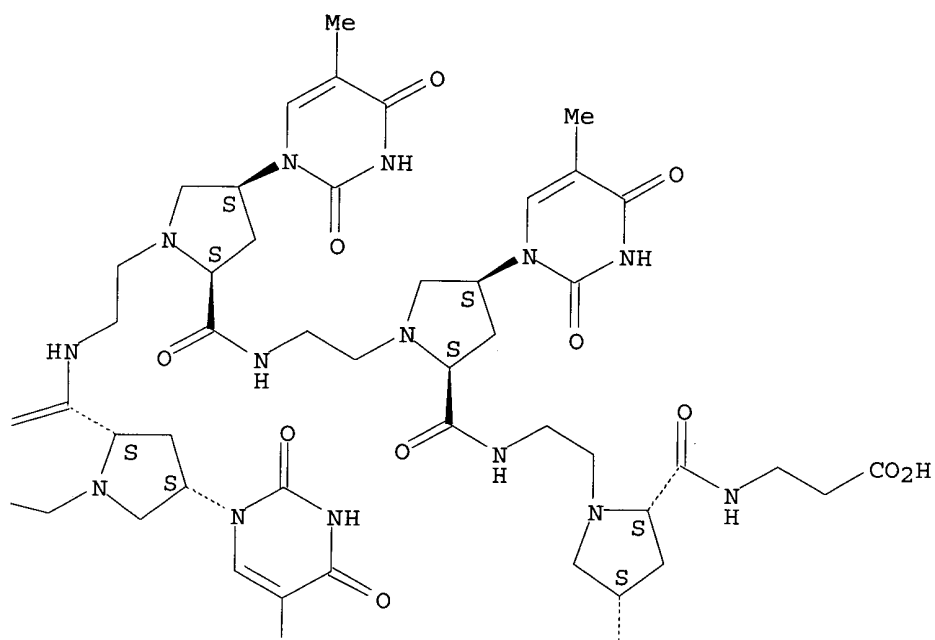
Absolute stereochemistry.

PAGE 1-A

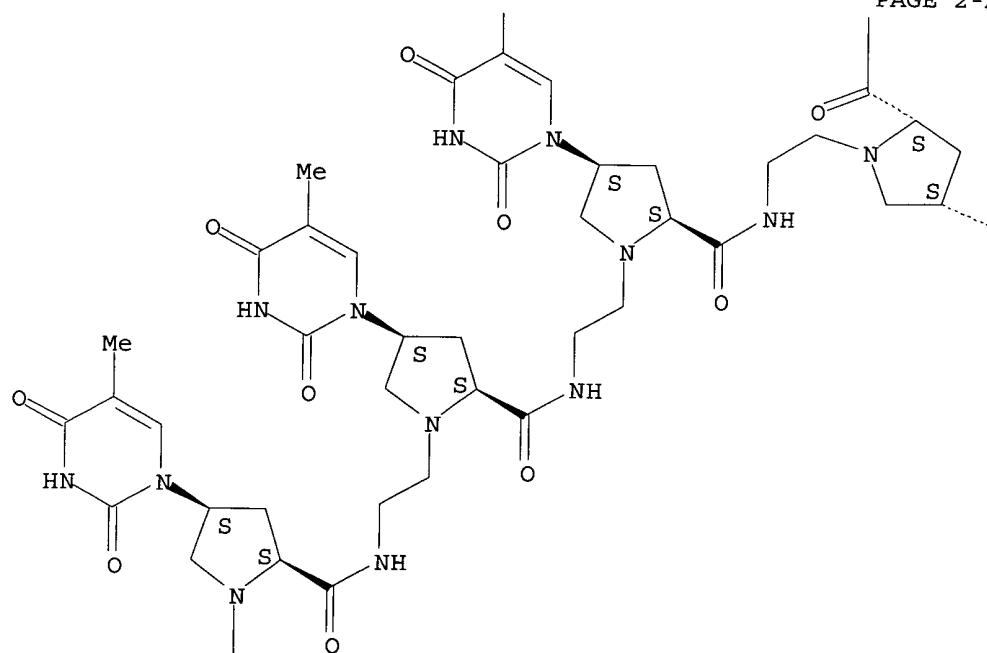
Me



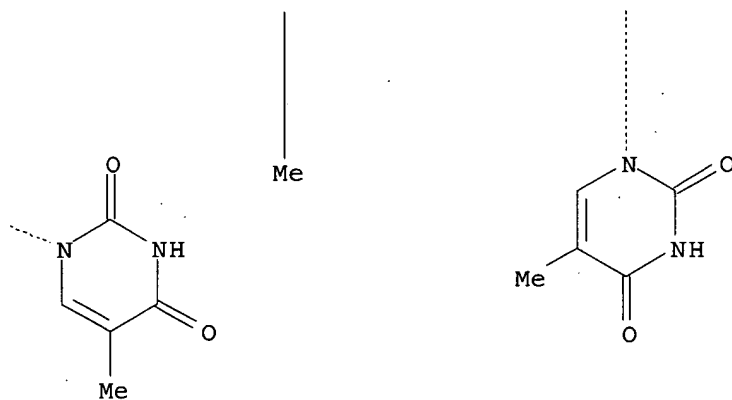
PAGE 1-B



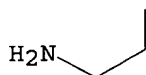
PAGE 2-A



PAGE 2-B



PAGE 3-A



RN 262615-78-1 HCAPLUS
 CN DNA, d(G-C-A-A-A-T-A-A-A-A-C-G), complex with peptide nucleic acid
 (H-T- (4S) -1- (2-aminoethyl) -4- (3,4-dihydro-5-methyl-2,4-dioxo-1(2H) -
 pyrimidinyl) -D-Pro-T- (4S) -1- (2-aminoethyl) -4- (3,4-dihydro-5-methyl-2,4-
 dioxo-1(2H) -pyrimidinyl) -D-Pro-T- (4S) -1- (2-aminoethyl) -4- (3,4-dihydro-5-
 methyl-2,4-dioxo-1(2H) -pyrimidinyl) -D-Pro-T- (4S) -1- (2-aminoethyl) -4- (3,4-
 dihydro-5-methyl-2,4-dioxo-1(2H) -pyrimidinyl) -D-Pro) -Bal-OH (1:2) (9CI)
 (CA INDEX NAME)

CM 1

CRN 262408-14-0
 CMF Unspecified
 CCI MAN

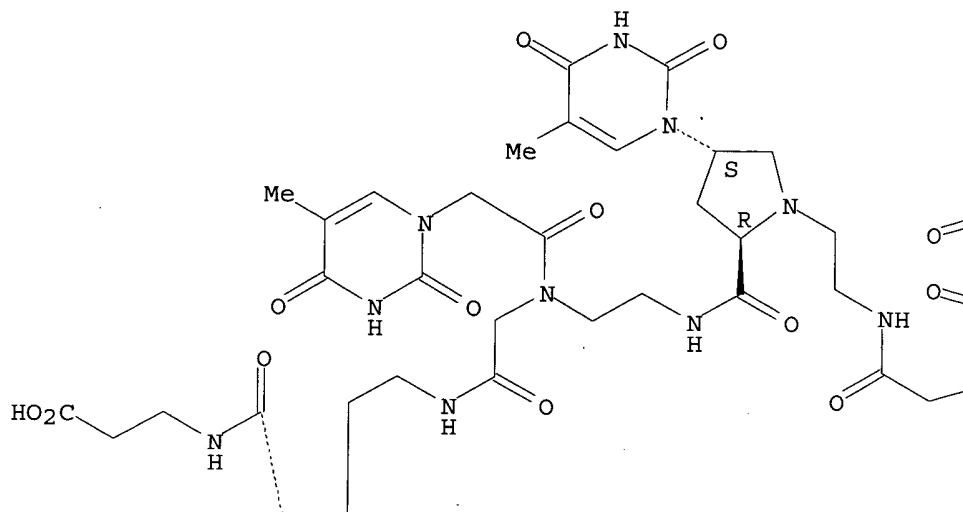
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CM 2

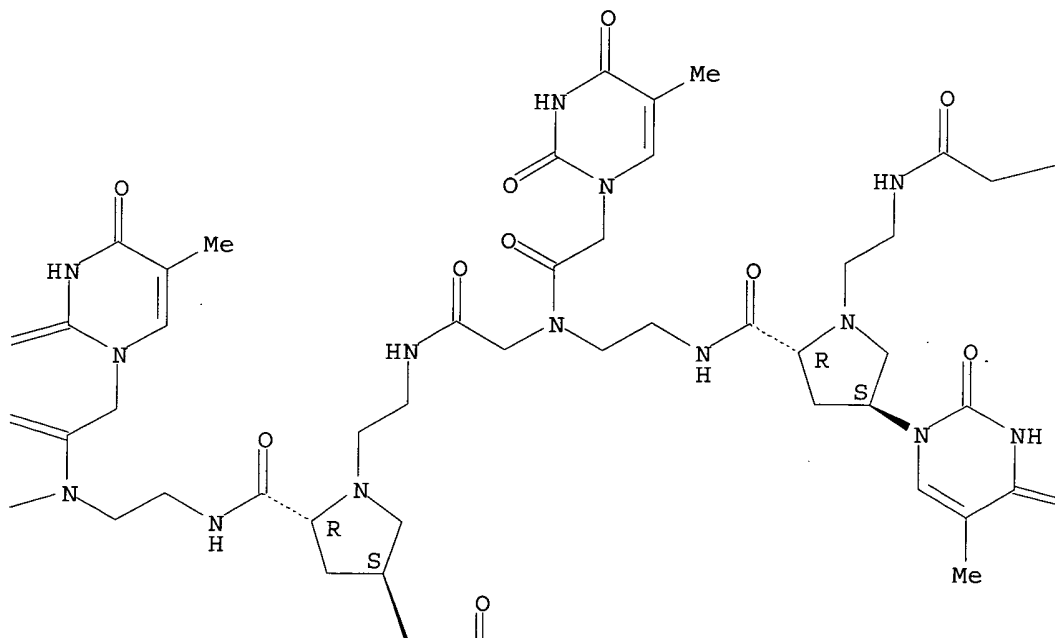
CRN 253342-10-8
 CMF C95 H127 N33 O30

Absolute stereochemistry.

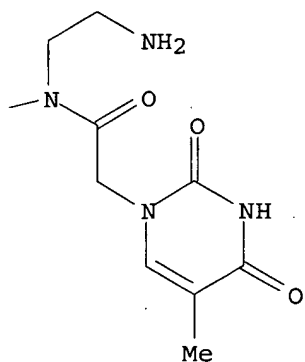
PAGE 1-A



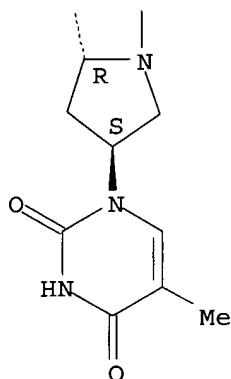
PAGE 1-B



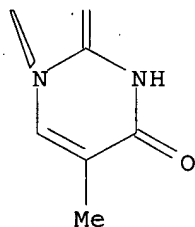
PAGE 1-C



PAGE 2-A



PAGE 2-B



RN 262615-79-2 HCAPLUS
 CN DNA, d(G-C-A-A-A-T-A-A-A-A-C-G), complex with peptide nucleic acid
 (H-T- (4S) -1- (2-aminoethyl) -4- (3,4-dihydro-5-methyl-2,4-dioxo-1(2H) -
 pyrimidinyl) -Pro-T- (4S) -1- (2-aminoethyl) -4- (3,4-dihydro-5-methyl-2,4-dioxo-
 1(2H) -pyrimidinyl) -Pro-T- (4S) -1- (2-aminoethyl) -4- (3,4-dihydro-5-methyl-2,4-

dioxo-1(2H)-pyrimidinyl)-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pro)-Bal-OH (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 262408-14-0

CMF Unspecified

CCI MAN

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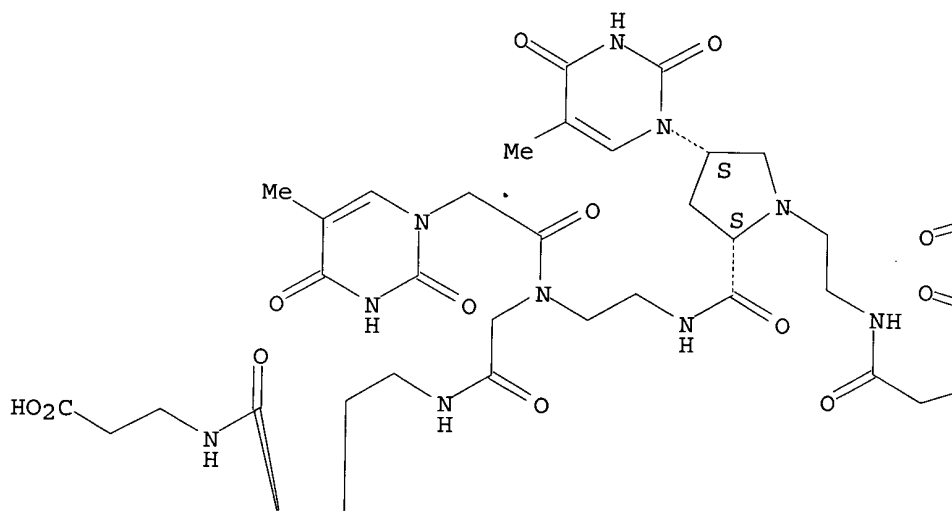
CM 2

CRN 253342-11-9

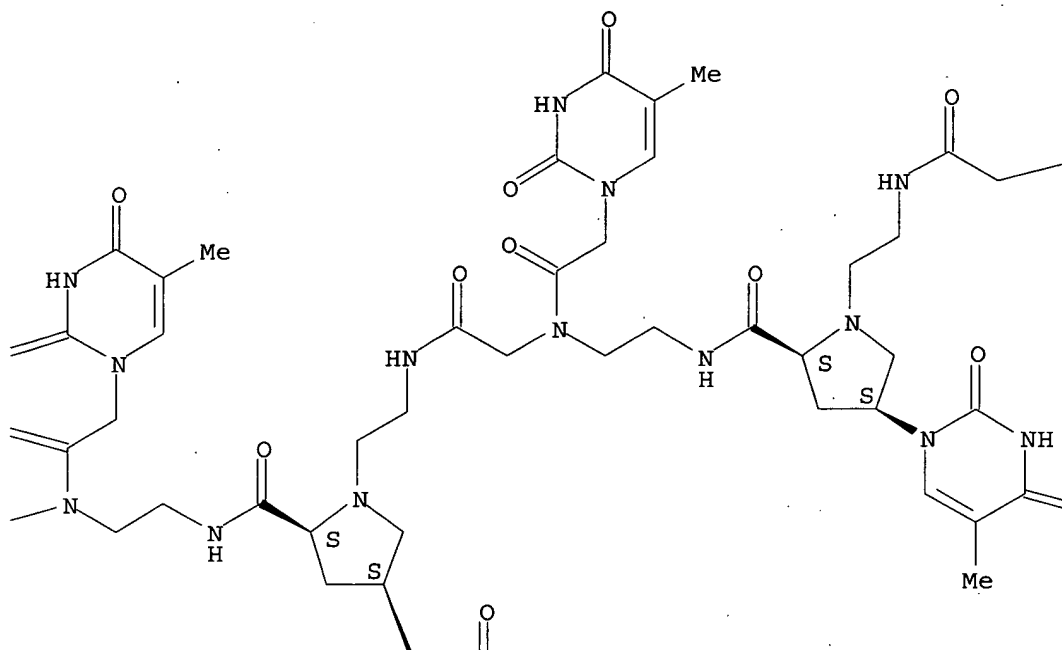
CMF C95 H127 N33 O30

Absolute stereochemistry.

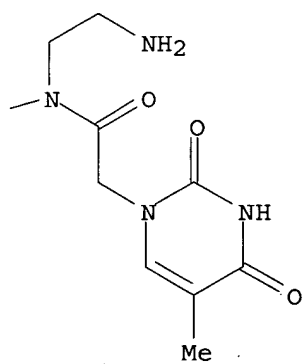
PAGE 1-A



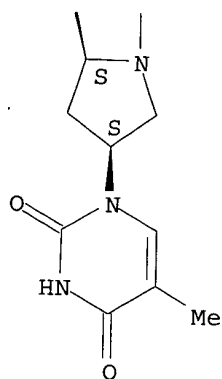
PAGE 1-B



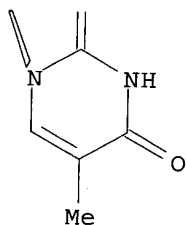
PAGE 1-C



PAGE 2-A



PAGE 2-B



RN 262615-84-9 HCAPLUS
 CN DNA, d(G-C-A-A-A-T-A-A-A-C-G), complex with peptide nucleic acid
 (H-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-
 pyrimidinyl)-D-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-
 1(2H)-pyrimidinyl)-D-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-
 dioxo-1(2H)-pyrimidinyl)-D-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-
 methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-
 dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-(4S)-1-(2-aminoethyl)-
 4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-(4S)-1-(2-
 aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-
 (4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-
 D-Pro)-Bal-OH (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 262408-14-0
 CMF Unspecified
 CCI MAN

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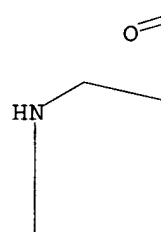
CM 2

CRN 253342-12-0
 CMF C99 H135 N33 O26

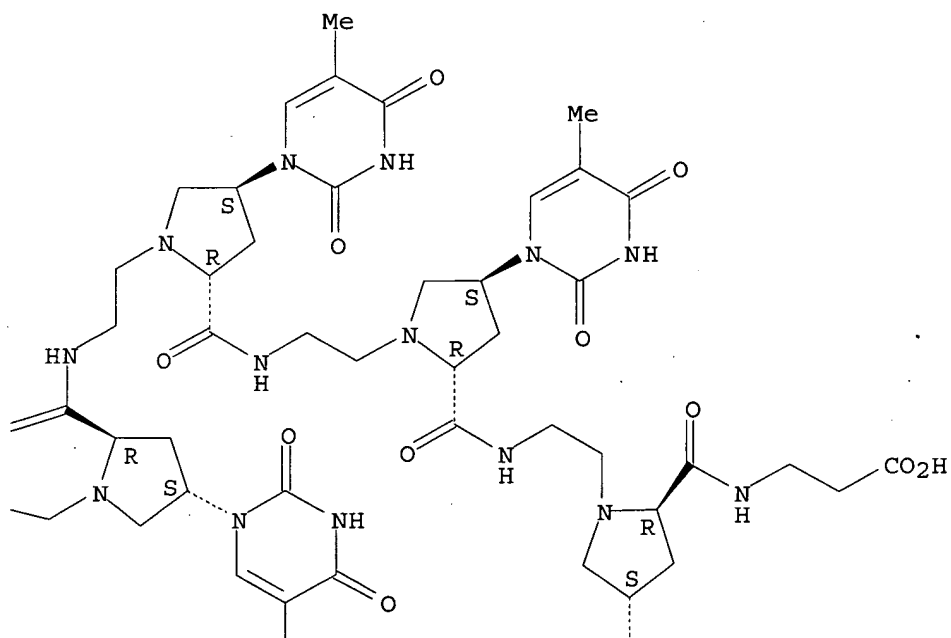
Absolute stereochemistry.

PAGE 1-A

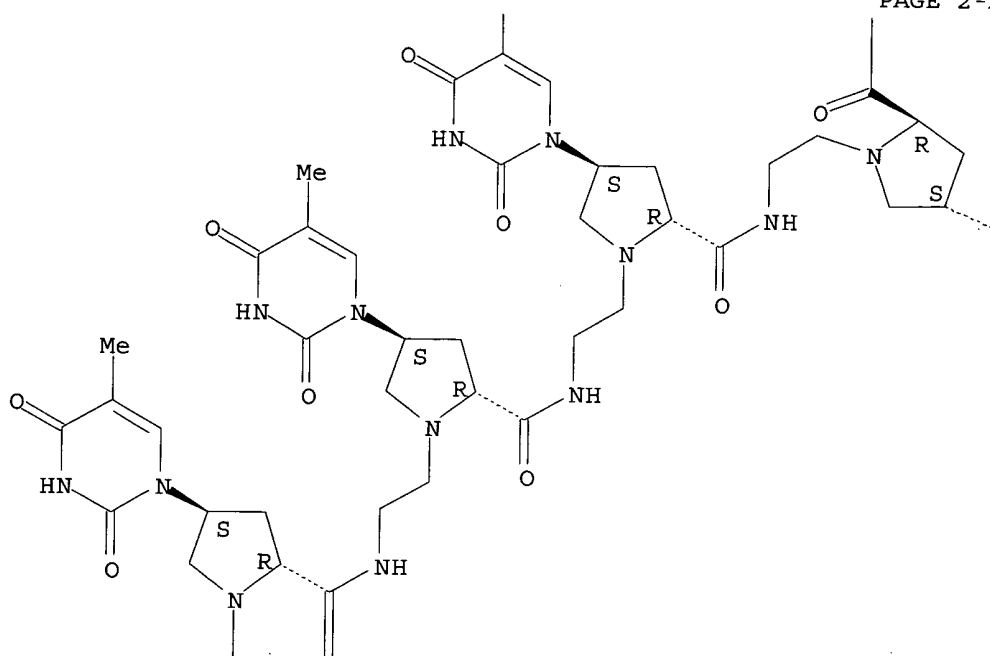
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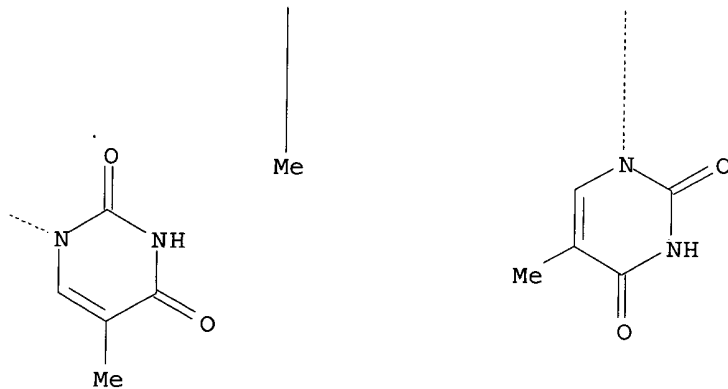
PAGE 1-B



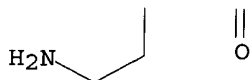
PAGE 2-A



PAGE 2-B



PAGE 3-A



RN 262615-88-3 HCAPLUS
 CN DNA, d(G-C-A-A-A-T-A-A-A-C-G), complex with peptide nucleic acid
 (H-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-
 pyrimidinyl)-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-
 1(2H)-pyrimidinyl)-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-

dioxo-1(2H)-pyrimidinyl)-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pro)-Bal-OH (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 262408-14-0

CMF Unspecified

CCI MAN

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

CM 2

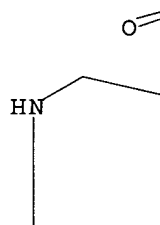
CRN 253342-13-1

CMF C99 H135 N33 O26

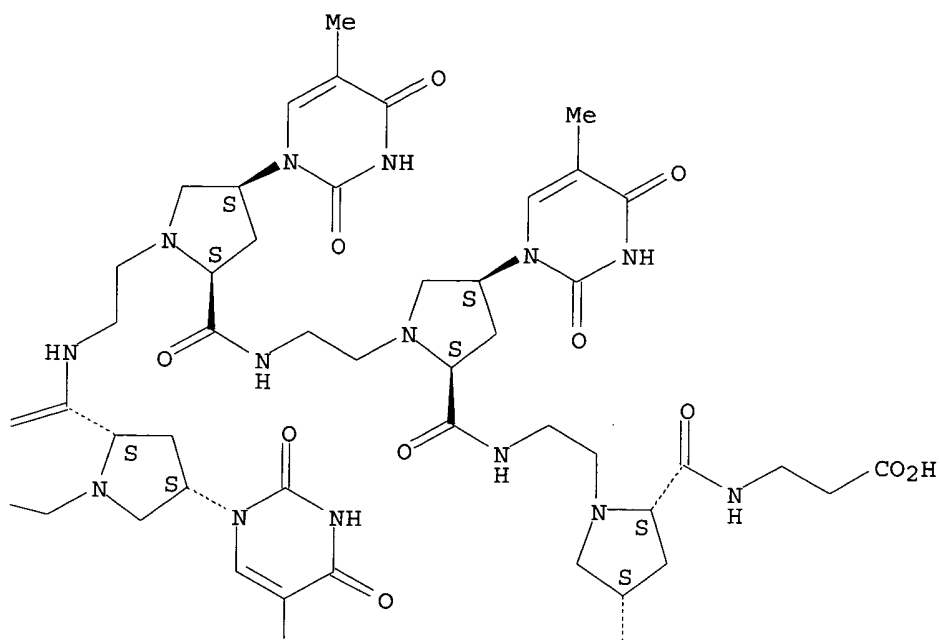
Absolute stereochemistry.

PAGE 1-A

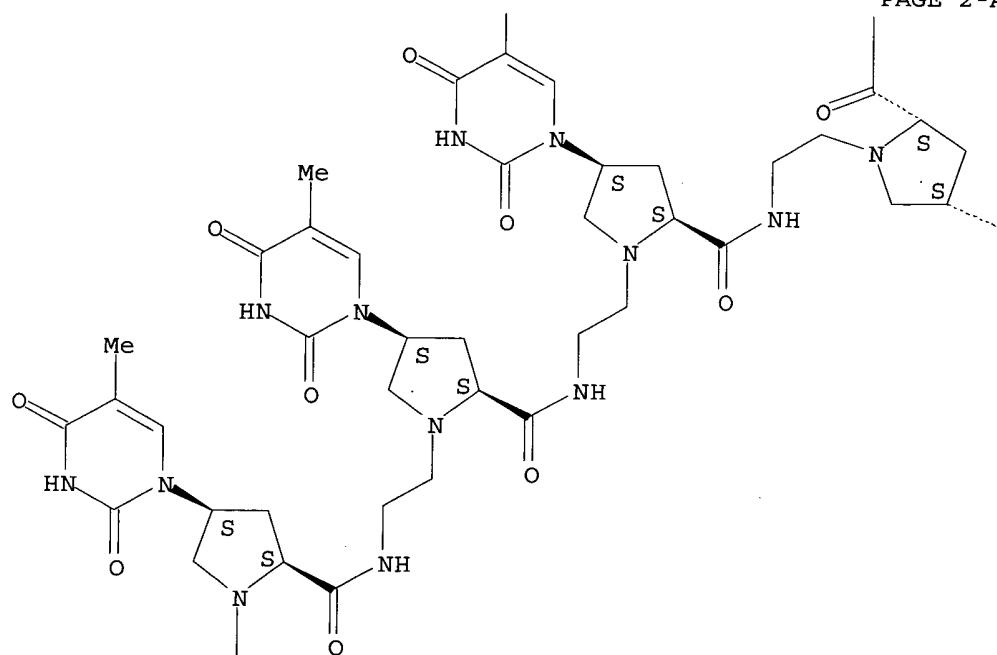
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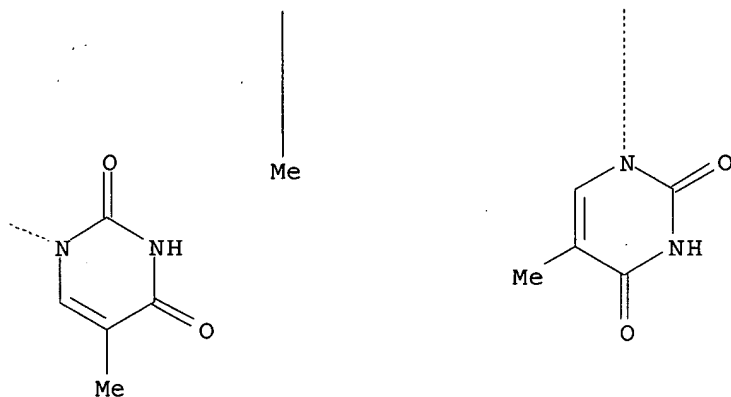
PAGE 1-B



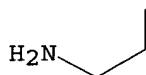
PAGE 2-A



PAGE 2-B



PAGE 3-A



RN 262615-89-4 HCAPLUS
CN DNA, d(G-C-A-A-A-A-A-A-A-A-C-G), complex with peptide nucleic acid
(H-T-T-T-T-T-T-T-T)-β-ala-OH (1:2) (9CI) (CA INDEX NAME)

CM 1

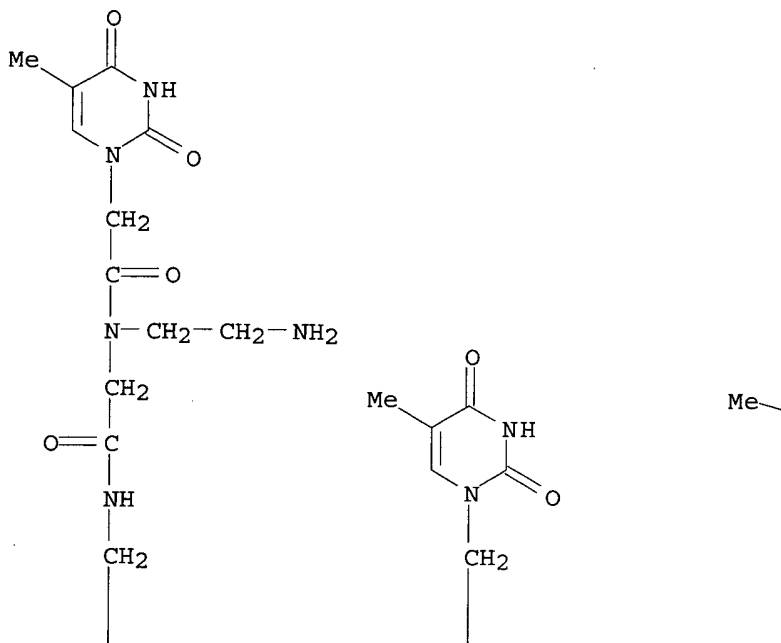
CRN 262408-13-9
CMF Unspecified
CCI MAN

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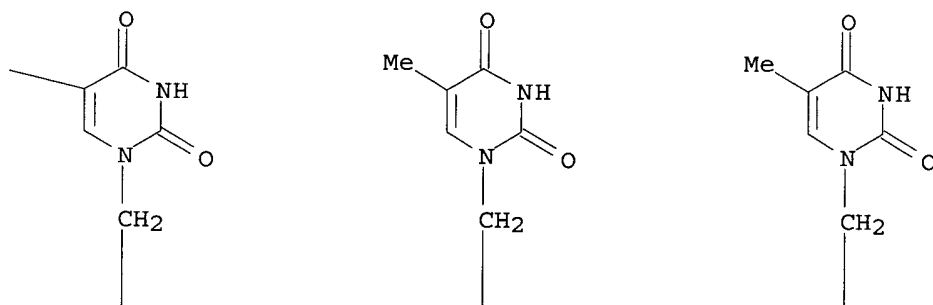
CM 2

CRN 253307-86-7
CMF C91 H119 N33 O34

PAGE 1-A



PAGE 1-B

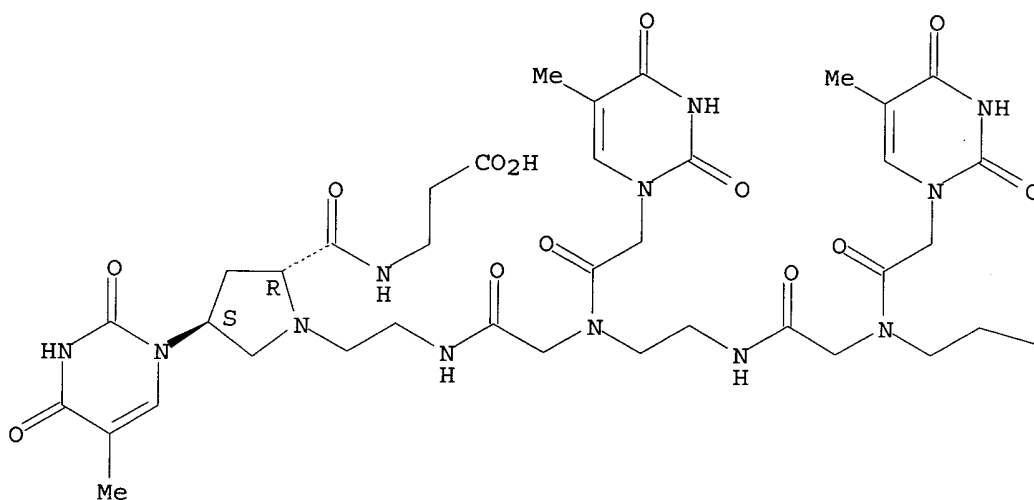


Cc1cc(C(=O)NCC(=O)NCCC(=O)O)cnc1C(=O)N[illegible]
$$\begin{array}{ccccccc} & | & & & | & & | \\ & \text{O}=\text{C} & & & \text{C}=\text{O} & & \text{C}=\text{O} \\ & | & & & | & & | \\ -\text{CH}_2- & \text{N}-\text{CH}_2-\text{C}(=\text{O})-\text{NH}- & \text{CH}_2-\text{CH}_2-\text{N}-\text{CH}_2-\text{C}(=\text{O})-\text{NH}- & \text{CH}_2-\text{CH}_2-\text{N}-\text{CH}_2-\text{C}(=\text{O})-\text{NH}- \end{array}$$
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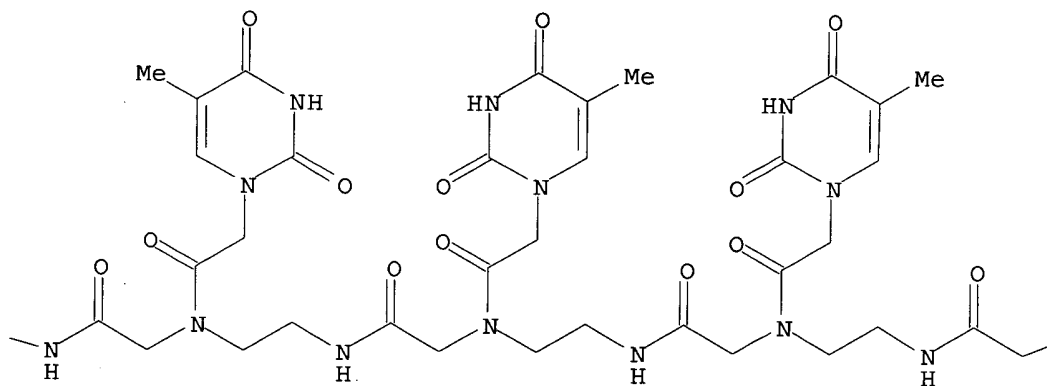
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253307-84-5P 253342-10-8P 253342-11-9P
253342-12-0P 253342-13-1P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and triplex-forming properties of as chiral PNA analogs)
RN 253307-78-7 HCAPLUS
CN Peptide nucleic acid, (H-T-T-T-T-T-T-T-(4S)-1-(2-aminoethyl)-4-(3,4-
dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro)-Bal-OH (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

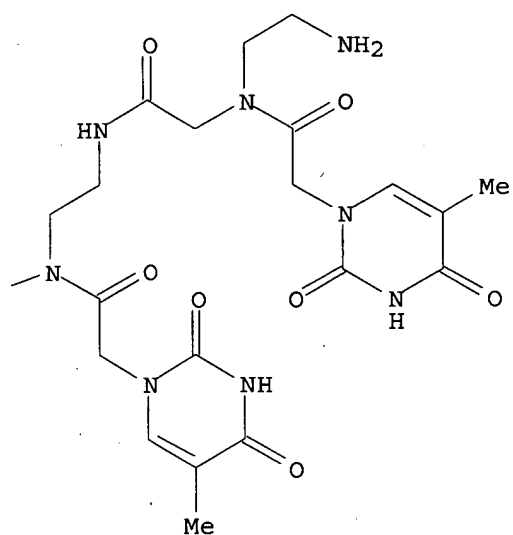
PAGE 1-A



PAGE 1-B



PAGE 1-C

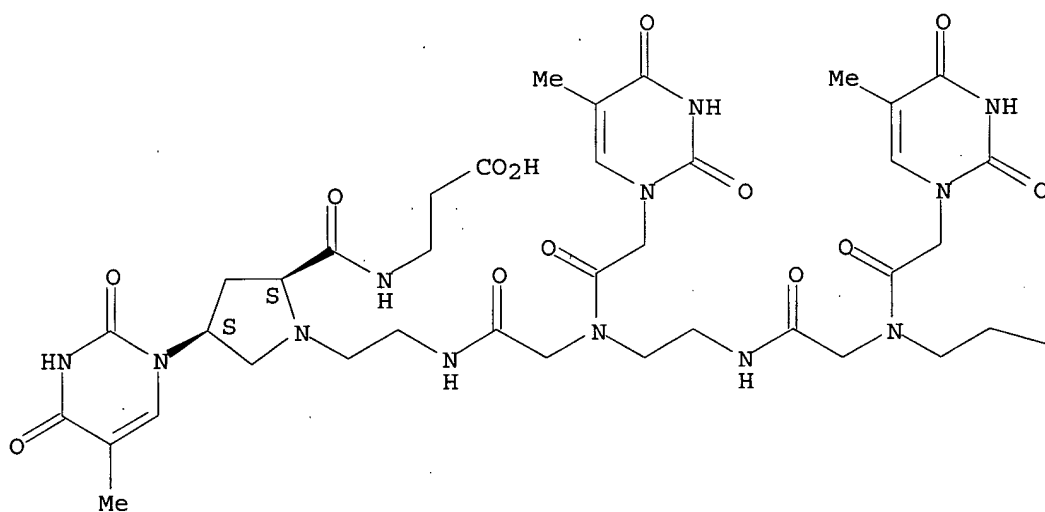


RN 253307-80-1 HCAPLUS

CN Peptide nucleic acid, (H-T-T-T-T-T-T-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pro)-Bal-OH (9CI) (CA INDEX NAME)

Absolute stereochemistry.

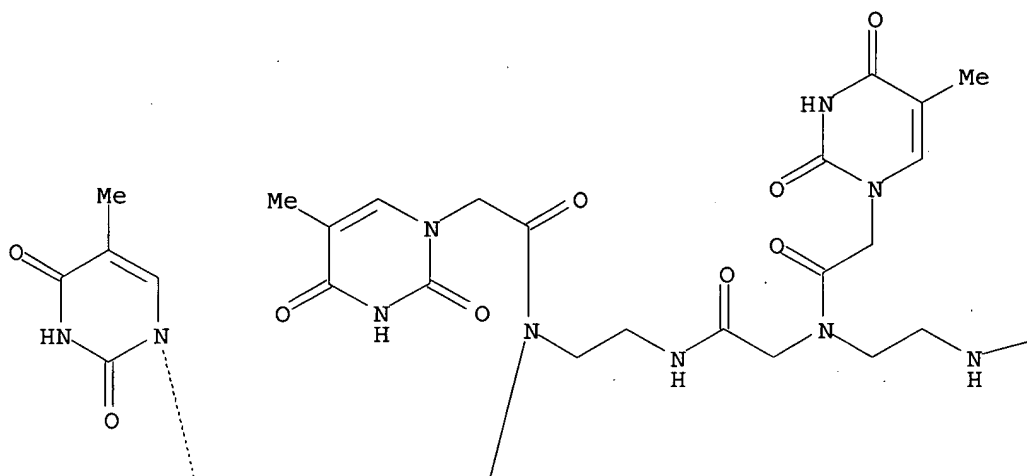
PAGE 1-A



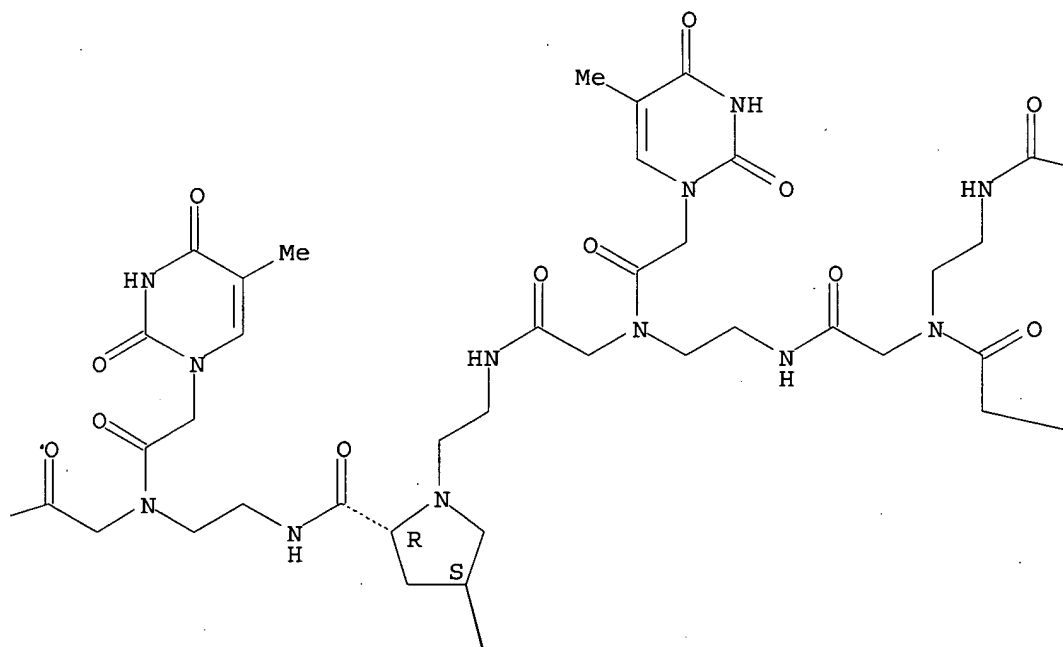
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Absolute stereochemistry.

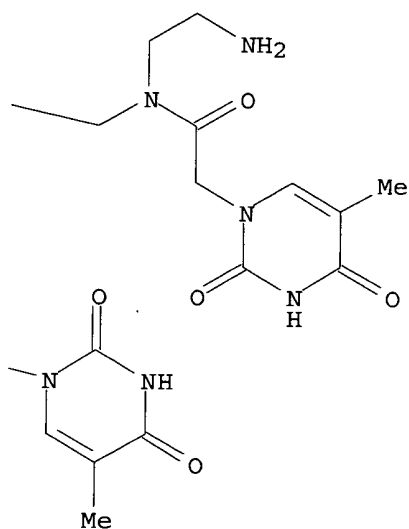
PAGE 1-A



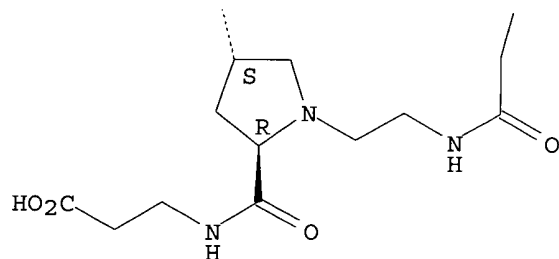
PAGE 1-B



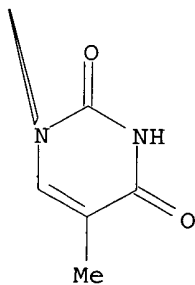
PAGE 1-C



PAGE 2-A



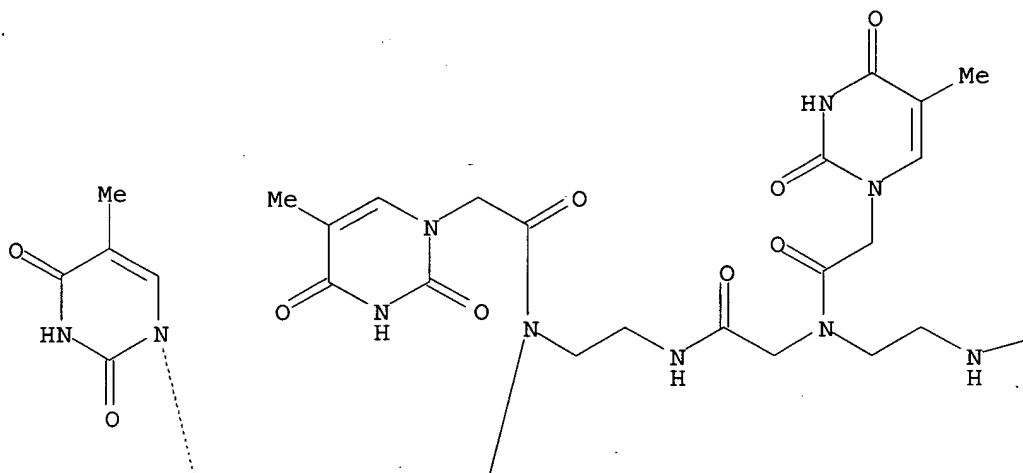
PAGE 2-B



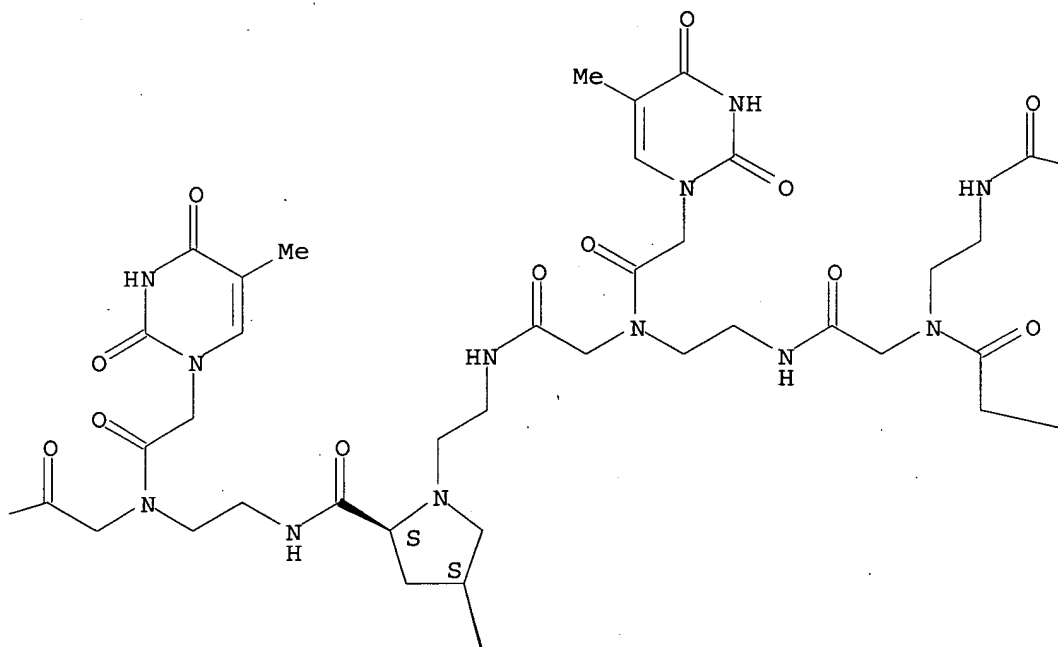
RN 253307-84-5 HCAPLUS
 CN Peptide nucleic acid, (H-T-T-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pro-T-T-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pro)-Bal-OH (9CI) (CA INDEX NAME)

Absolute stereochemistry.

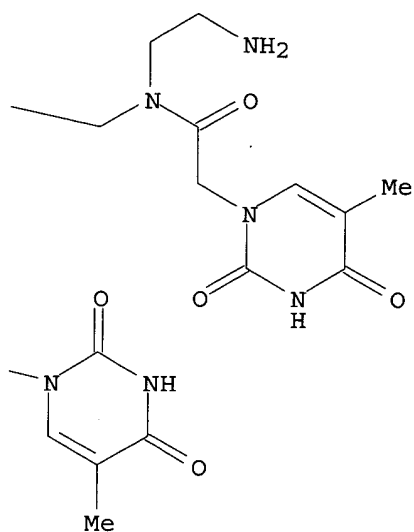
PAGE 1-A



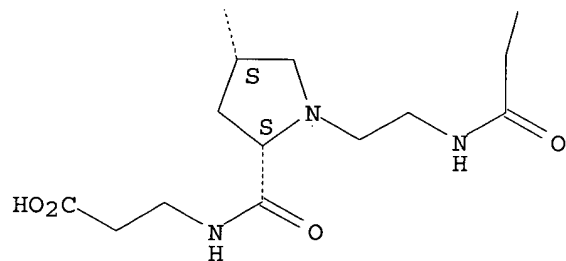
PAGE 1-B



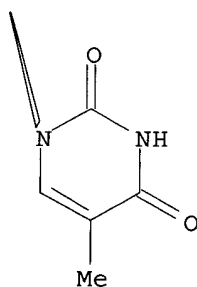
PAGE 1-C



PAGE 2-A



PAGE 2-B

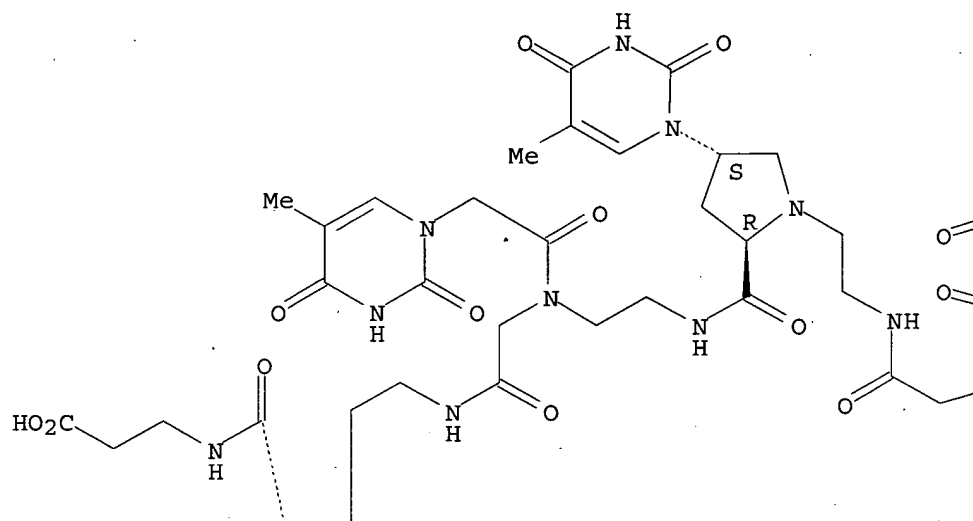


RN 253342-10-8 HCAPLUS
 CN Peptide nucleic acid, (H-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-T-(4S)-1-(2-

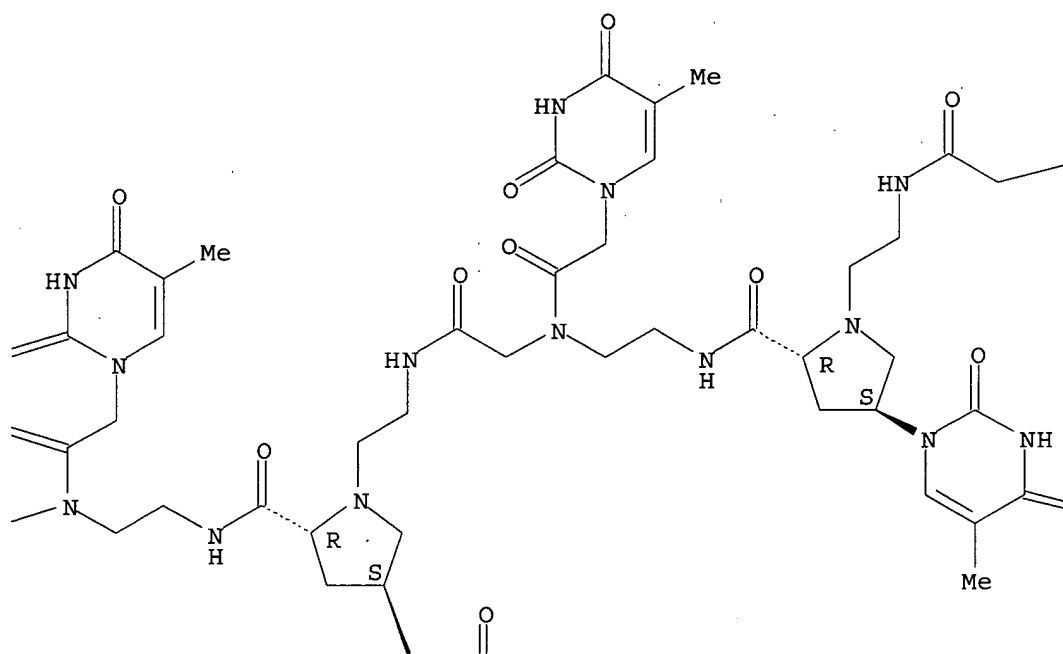
aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro)-
Bal-OH (9CI) (CA INDEX NAME)

Absolute stereochemistry.

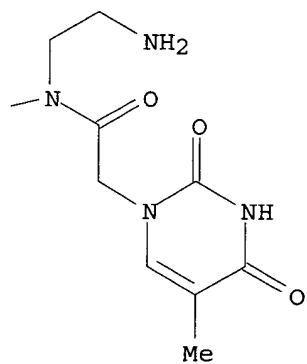
PAGE 1-A



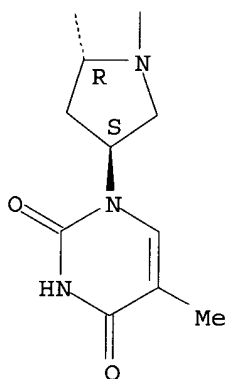
PAGE 1-B



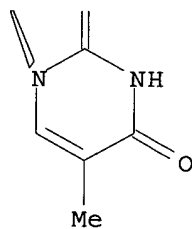
PAGE 1-C



PAGE 2-A



PAGE 2-B

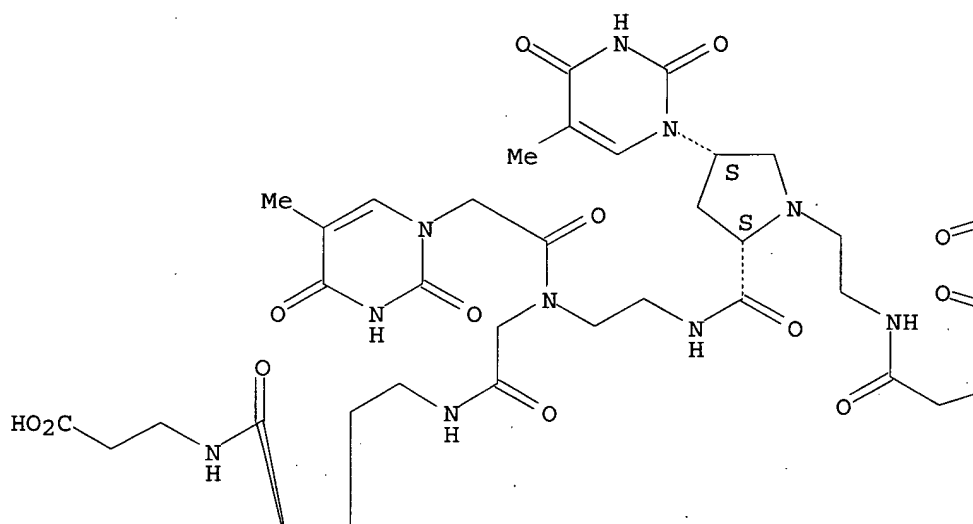


RN 253342-11-9 HCAPLUS
 CN Peptide nucleic acid, (H-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-

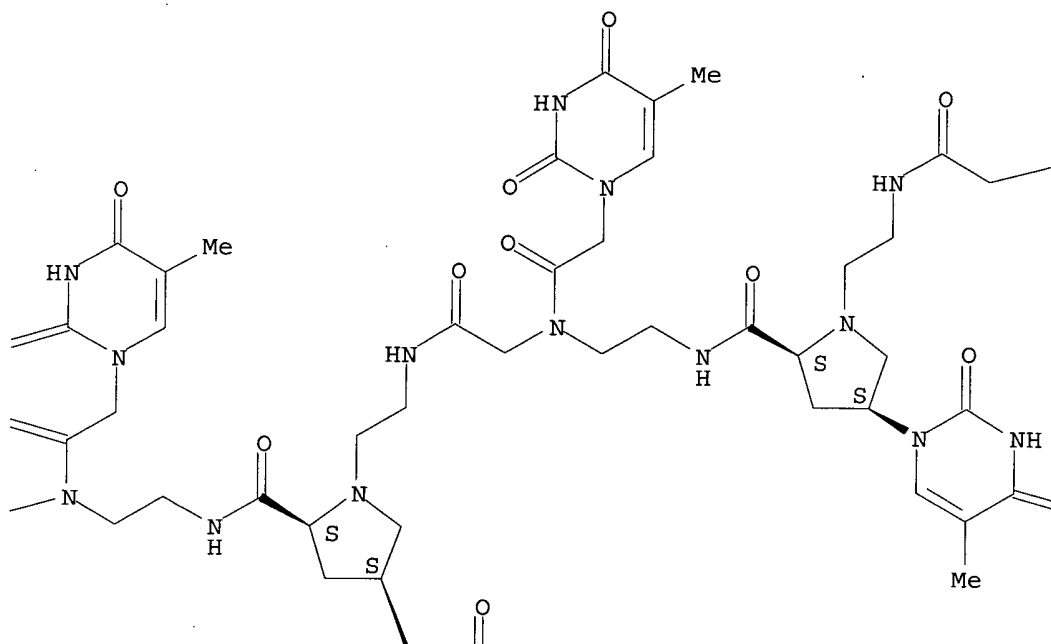
methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pro-T-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pro)-Bal-OH (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

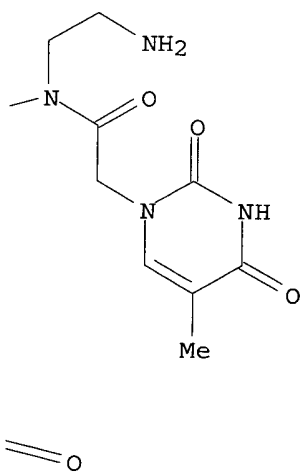
PAGE 1-A



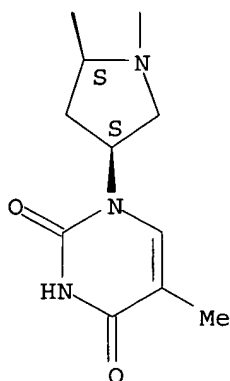
PAGE 1-B



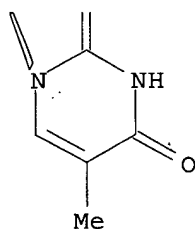
PAGE 1-C



PAGE 2-A



PAGE 2-B



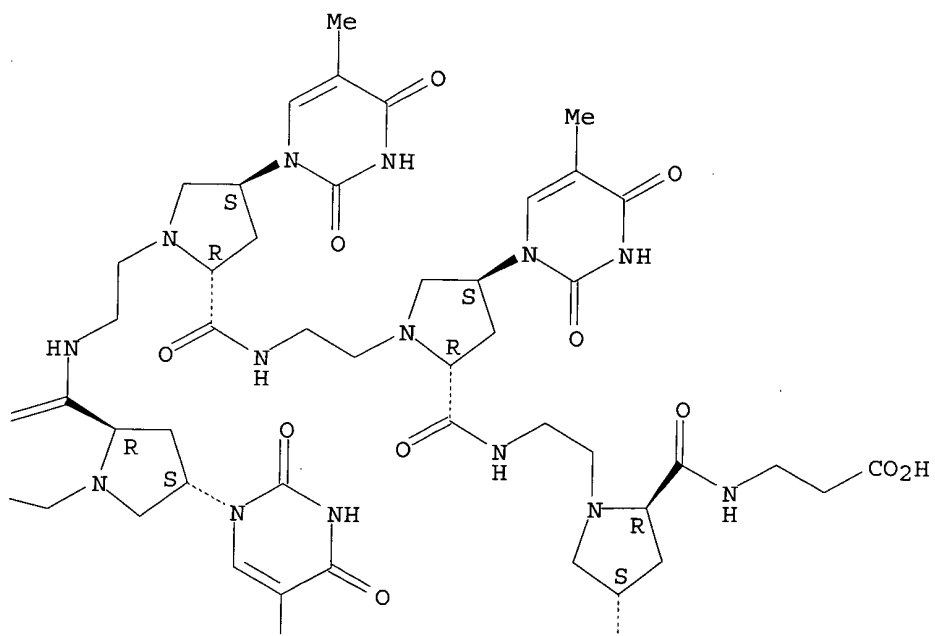
RN 253342-12-0 HCAPLUS
 CN Peptide nucleic acid, (H-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-D-Pro)-Bal-OH (9CI) (CA INDEX NAME)

Absolute stereochemistry.

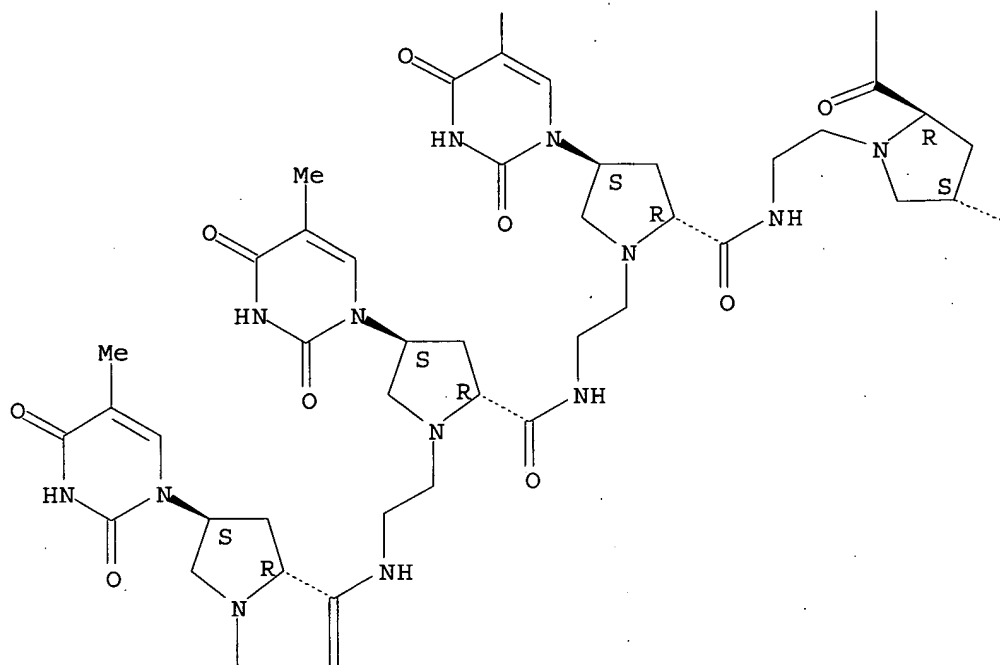
PAGE 1-A



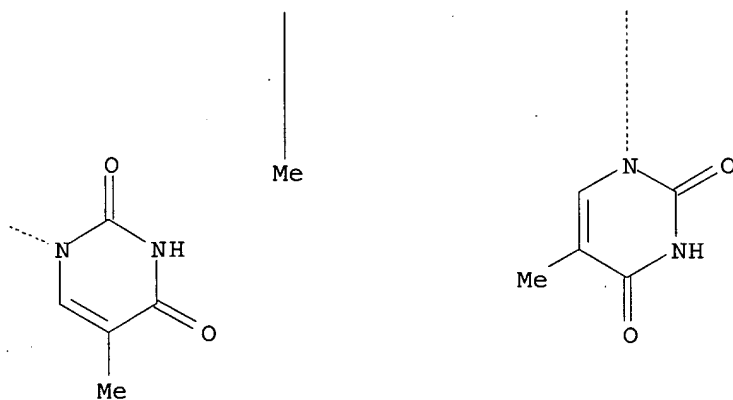
PAGE 1-B



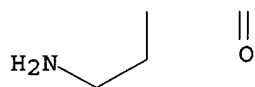
PAGE 2-A



PAGE 2-B



PAGE 3-A



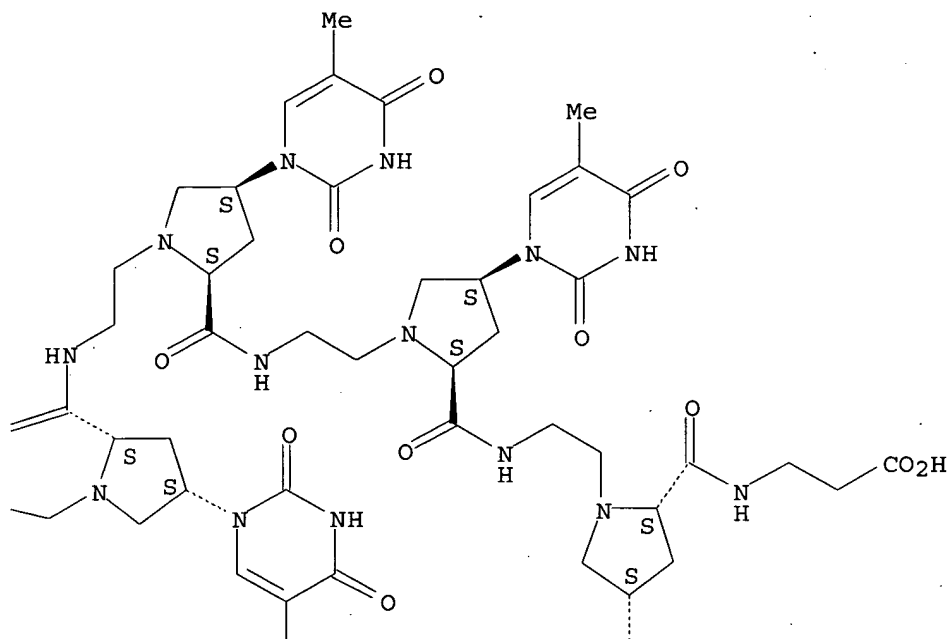
RN 253342-13-1 HCAPLUS
 CN Peptide nucleic acid, (H-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-Pro-(4S)-1-(2-aminoethyl)-4-(3,4-

Absolute stereochemistry.

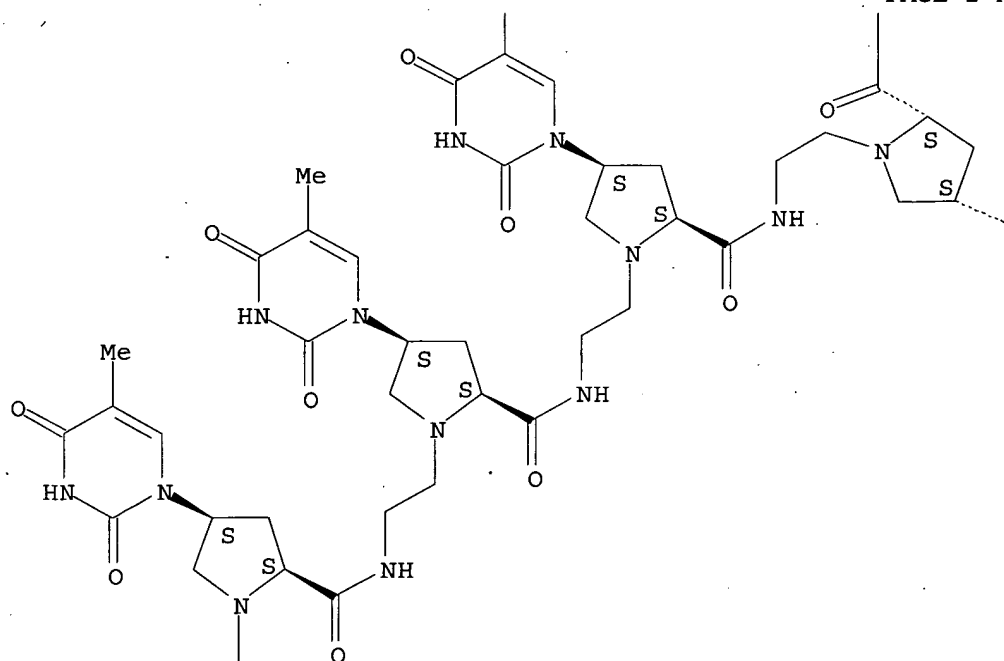
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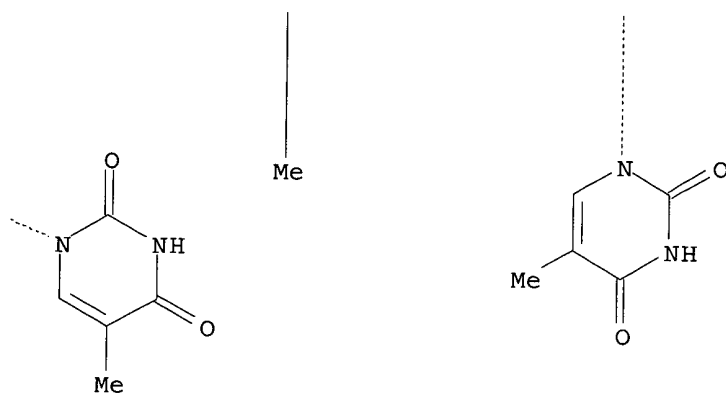
PAGE 1-B



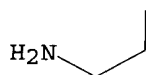
PAGE 2-A



PAGE 2-B



PAGE 3-A



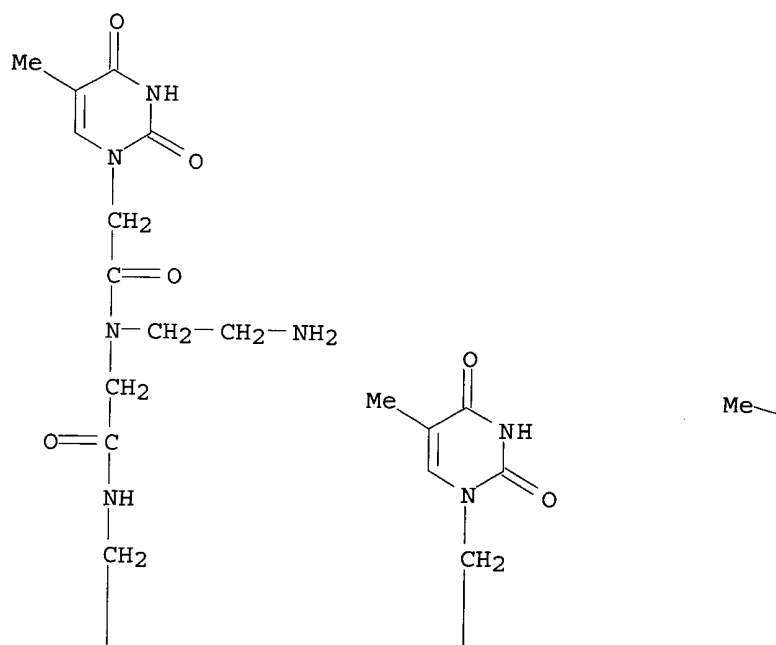
IT 253307-86-7P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (preparation and triplex-forming properties of as comparison for chiral PNA
 analogs)

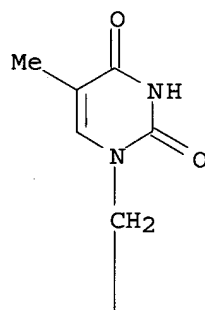
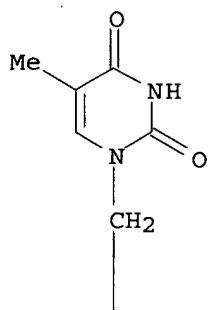
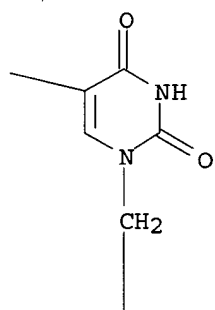
RN 253307-86-7 HCAPLUS

CN Peptide nucleic acid, (H-T-T-T-T-T-T-T)-β-ala-OH (9CI) (CA INDEX
 NAME)

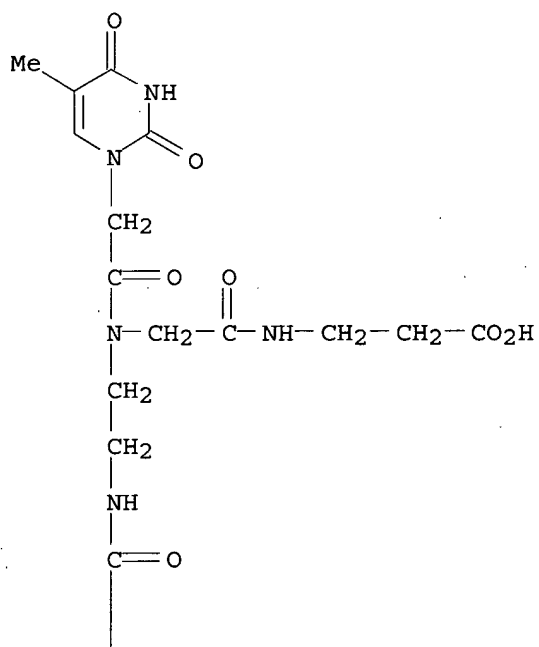
PAGE 1-A



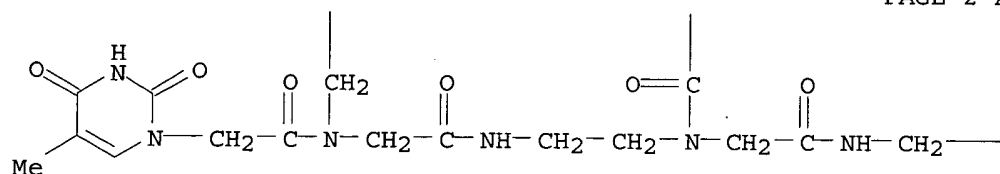
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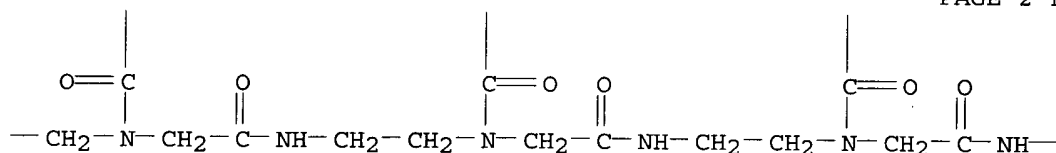
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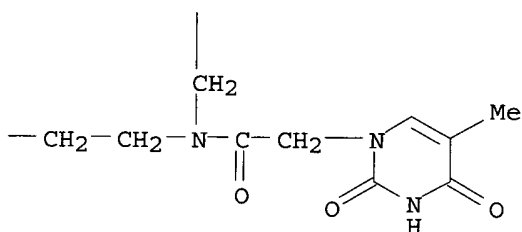
PAGE 2-A



PAGE 2-B



PAGE 2-C



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L38 ANSWER 11 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1971:488556 HCAPLUS

DOCUMENT NUMBER: 75:88556

TITLE: Neuroleptic phenothiazines with 1,4-diazabicyclo[4.4.0]decane and [4.3.0]nonane ring system

AUTHOR(S): Casagrande, C.; Galli, A.; Ferrini, R.; Miragoli, G.

CORPORATE SOURCE: Res. Lab., Simes S.p.A., Milan, Italy

SOURCE: Arzneimittel-Forschung (1971), 21(6), 808-11

CODEN: ARZNAD; ISSN: 0004-4172

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB 4-[γ-(2-Trifluoromethyl-10-phenothiazinyl)propyl]-10-hydroxymethyl-1,4-diazabicyclo[4.4.0]decane (I), 4-[γ-(2-trifluoromethyl-10-phenothiazinyl)propyl]-1,4-diazabicyclo[4.4.0]decane, 4-[γ-(2-chloro-10-phenothiazinyl)propyl]-1,4-diazabicyclo[4.4.0]decane, 4-[γ-(10-phenothiazinyl)propyl]-1,4-diazabicyclo[4.4.0]decane, and 4-[γ-(2-trifluoromethyl-10-phenothiazinyl)propyl]-1,4-diazabicyclo[4.3.0]nonane were prepared by alkylating the secondary N of the appropriate diazabicyclic derivs. with 10-(γ-chloropropyl)phenothiazines and 4-[γ-5-(10,11-dihydro-5H-dibenzo[a,d]cycloheptenylidene)propyl]-1,4-diazabicyclo[4.4.0]decane (II)

was obtained similarly from 5-(γ -bromopropylidene)-10,11-dihydro-5H-dibenzo[a,d]cycloheptene. I, the most active in a number of tests, pharmacol. resembled perphenazine. Structureactivity relations were briefly discussed.

CC 28 (Heterocyclic Compounds (More Than One Hetero Atom))

IT 274-45-3DP, Pyrrolo[1,2-a]pyrazine, derivs. **33264-98-1P**

33264-99-2P 33492-19-2P 33492-20-5P 33492-21-6P 33492-22-7P

33492-23-8P

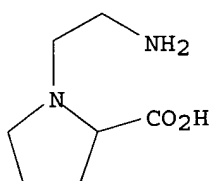
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT **33264-98-1P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 33264-98-1 HCAPLUS

CN Proline, 1-(2-aminoethyl)-, dihydrochloride, DL- (8CI) (CA INDEX NAME)



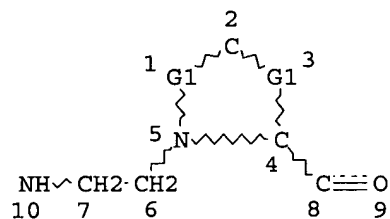
● 2 HCl

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L11

STR



REP G1=(1-2) CH2

NODE ATTRIBUTES:

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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

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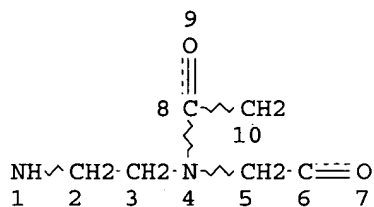
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STEREO ATTRIBUTES: NONE

L13 137 SEA FILE=REGISTRY SSS FUL L11

L14 2 SEA FILE=REGISTRY ABB=ON PLU=ON L13 AND PMS/CI

L16 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE

L18 2249 SEA FILE=REGISTRY SSS FUL L16

L19 26 SEA FILE=REGISTRY ABB=ON PLU=ON L18 AND L13

L20 3 SEA FILE=HCAPLUS ABB=ON PLU=ON L19

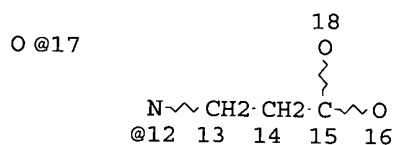
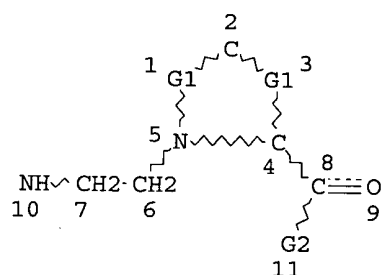
L21 6 SEA FILE=HCAPLUS ABB=ON PLU=ON L13 AND L18

L22 6 SEA FILE=HCAPLUS ABB=ON PLU=ON L20 OR L21

L23 1 SEA FILE=HCAPLUS ABB=ON PLU=ON L14

L24 7 SEA FILE=HCAPLUS ABB=ON PLU=ON L22 OR L23

L29 STR

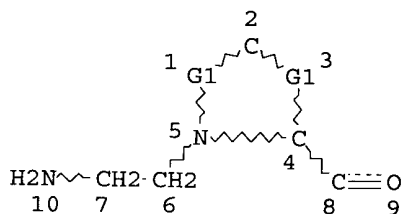


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 @19 20 21 22 23 24 25

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 CONNECT IS E1 RC AT 16
 CONNECT IS E1 RC AT 17
 CONNECT IS E1 RC AT 18
 CONNECT IS E2 RC AT 20
 CONNECT IS E2 RC AT 22
 CONNECT IS E2 RC AT 24
 DEFAULT MLEVEL IS ATOM
 GGCAT IS LIN LOC SAT AT 20
 GGCAT IS LIN LOC SAT AT 22
 GGCAT IS LIN LOC SAT AT 24
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 25

STEREO ATTRIBUTES: NONE
 L30 46 SEA FILE=REGISTRY SUB=L13 SSS FUL L29
 L31 STR

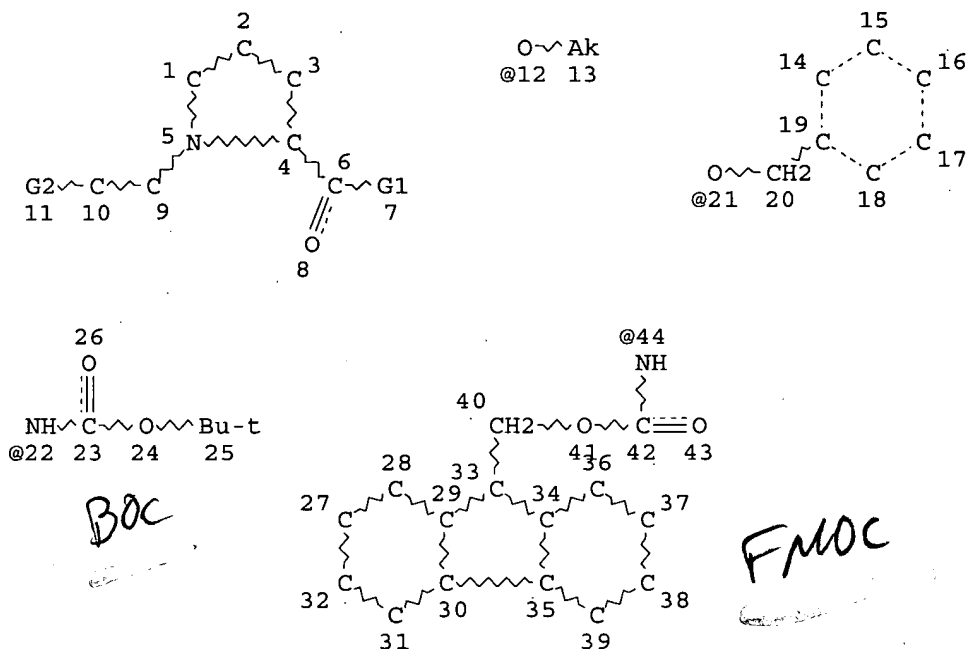


REP G1=(1-2) CH2
 NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE

L32 27 SEA FILE=REGISTRY SUB=L13 SSS FUL L31
 L33 8 SEA FILE=HCAPLUS ABB=ON PLU=ON L30 AND L32
 L34 14106 SEA FILE=HCAPLUS ABB=ON PLU=ON BIOTIN+PFT,NT/CT
 L35 24339 SEA FILE=HCAPLUS ABB=ON PLU=ON FLUORESCENT SUBSTANCES+PFT,NT/CT
 L36 2 SEA FILE=HCAPLUS ABB=ON PLU=ON L30 AND (L34 OR L35 OR BIOTIN OR FLUORES? OR FLUOROPHOR?)
 L38 11 SEA FILE=HCAPLUS ABB=ON PLU=ON L33 OR L36 OR L24
 L39 STR



VAR G1=H/12/21
 VAR G2=NH2/44/22
 NODE ATTRIBUTES:
 CONNECT IS E1 RC AT 13
 DEFAULT MLEVEL IS ATOM
 GGCAT IS LOC AT 13
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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 NUMBER OF NODES IS 44

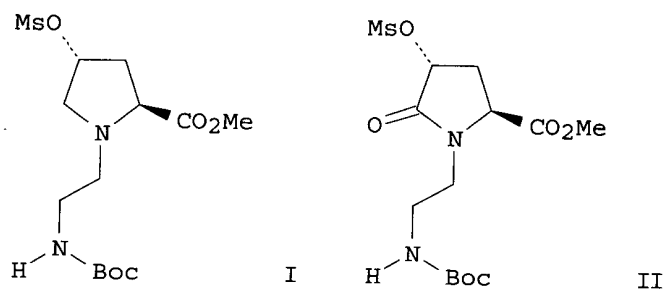
STEREO ATTRIBUTES: NONE

L40 31 SEA FILE=REGISTRY SUB=L13 SSS FUL L39
 L41 8 SEA FILE=HCAPLUS ABB=ON PLU=ON L40
 L42 2 SEA FILE=HCAPLUS ABB=ON PLU=ON L41 NOT L38

=> d l42 ibib abs hitstr 1-2

L42 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 2004:74758 HCAPLUS
 DOCUMENT NUMBER: 140:287230
 TITLE: Regioselective oxidation of N-alkylpyrrolidines to

AUTHOR(S): pyrrolidin-5-ones by RuCl₃/NaIO₄
 CORPORATE SOURCE: Sharma, Nagendra K.; Ganesh, Krishna N.
 SOURCE: Division of Organic Chemistry (Synthesis), National
 Chemical Laboratory, Pune, 411008, India
 PUBLISHER: Tetrahedron Letters (2004), 45(7), 1403-1406
 DOCUMENT TYPE: CODEN: TELEAY; ISSN: 0040-4039
 LANGUAGE: Elsevier Science B.V.
 Journal
 GI English



AB RuCl₃ and NaIO₄, under biphasic conditions, selectively oxidized the N α -endo-methylene group of pyrrolidines, e.g., I, to form pyrrolidinones, e.g., II, without affecting the exo-methylene group adjacent to the N-heteroatom.

IT 253307-68-5

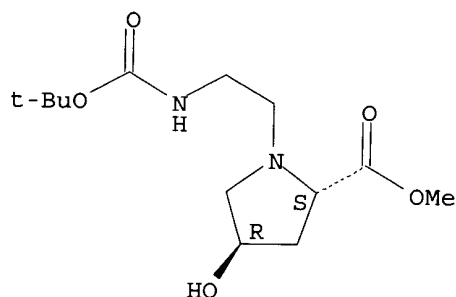
RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of O-protected N-alkyl(methoxycarbonyl)pyrrolidinols via O-protection of N-alkyl(methoxycarbonyl)pyrrolidinol with protecting groups in the preparation of N-alkyl(methoxycarbonyl)pyrrolidinones)

RN 253307-68-5 HCAPLUS

CN L-Proline, 1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-4-hydroxy-, methyl ester, (4R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 675824-92-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

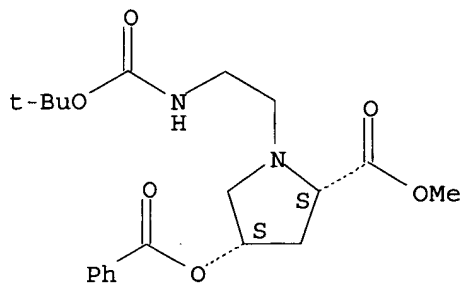
(regioselective preparation and crystal structure of N-(Boc-

aminoethyl)benzoyloxy(methoxycarbonyl)pyrrolidinone via
ruthenium-catalyzed oxidation of N-(Boc-aminoethyl)benzoyloxypyrrolidineca
rboxylate with sodium periodate)

RN 675824-92-7 HCAPLUS

CN L-Proline, 4-(benzoyloxy)-1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-
, methyl ester, (4S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



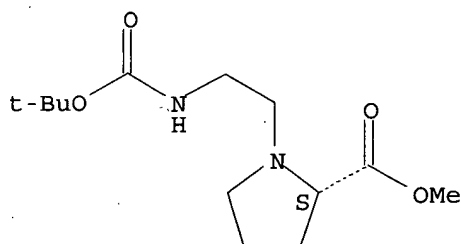
IT 675824-95-0

RL: RCT (Reactant); RACT (Reactant or reagent)
(regioselective preparation of N-(Boc-aminoethyl)(methoxycarbonyl)pyrrolidin
one via ruthenium-catalyzed oxidation of N-(Boc-
aminoethyl)pyrrolidinecarboxylate with sodium periodate)

RN 675824-95-0 HCAPLUS

CN L-Proline, 1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, methyl ester
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 340961-32-2P 675824-90-5P 675824-91-6P

675824-93-8P 675824-94-9P

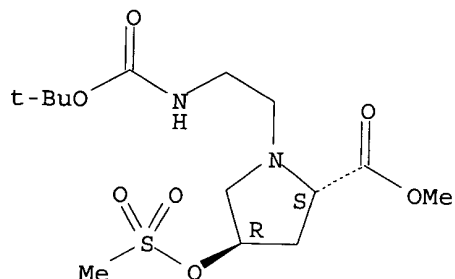
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(regioselective preparation of O-protected N-alkyl(methoxycarbonyl)pyrrolidi
nones via ruthenium-catalyzed oxidation of O-protected
N-alkyl(methoxycarbonyl)pyrrolidinols with sodium periodate)

RN 340961-32-2 HCAPLUS

CN L-Proline, 1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-4-
[(methylsulfonyl)oxy]-, methyl ester, (4R)-(9CI) (CA INDEX NAME)

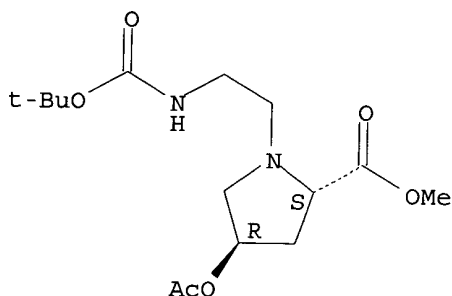
Absolute stereochemistry.



RN 675824-90-5 HCAPLUS

CN L-Proline, 4-(acetyloxy)-1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, methyl ester, (4R)- (9CI) (CA INDEX NAME)

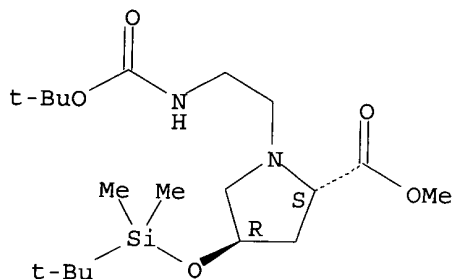
Absolute stereochemistry.



RN 675824-91-6 HCAPLUS

CN L-Proline, 1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-4-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-, methyl ester, (4R)- (9CI) (CA INDEX NAME)

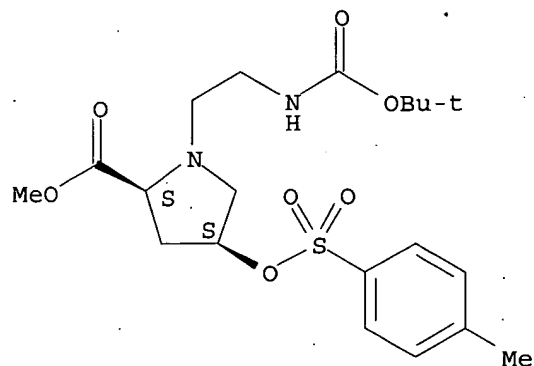
Absolute stereochemistry.



RN 675824-93-8 HCAPLUS

CN L-Proline, 1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-4-[[[(4-methylphenyl)sulfonyl]oxy]-, methyl ester, (4S)- (9CI) (CA INDEX NAME)

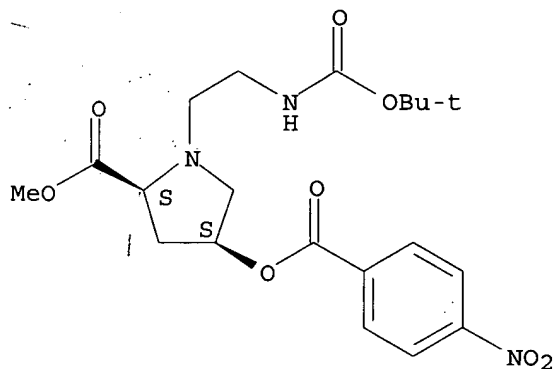
Absolute stereochemistry.



RN 675824-94-9 HCAPLUS

CN L-Proline, 1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-4-[(4-nitrobenzoyl)oxy]-, methyl ester, (4S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L42 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:238460 HCAPLUS

DOCUMENT NUMBER: 135:107554

TITLE: Aminoethylprolyl (aep) PNA: Mixed Purine/Pyrimidine Oligomers and Binding Orientation Preferences for PNA:DNA Duplex Formation

AUTHOR(S): D'Costa, Moneesha; Kumar, Vijayanti; Ganesh, Krishna N.

CORPORATE SOURCE: Division of Organic Chemistry (Synthesis), National Chemical Laboratory, Pune, 411008, India

SOURCE: Organic Letters (2001), 3(9), 1281-1284

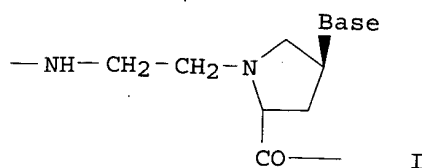
CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB The synthesis of (2S,4S)- and (2R,4S)-aepPNA monomers (I; Base = adenine, guanine, and cytosine) and their incorporation at appropriate positions into aegPNA sequence leads to mixed aeg-aep backbone/mixed nucleobase PNAs. Beginning with (2S,4R)-4-hydroxyl-N-(N-Boc-aminoethyl)-L-proline Me ester (Boc = (CH₃)₃COC(O)-) or its 2R,4R isomer, the hydroxy group was mesylated, and the product reacted with protected Base to give Boc-protected Me esters of I, which, with the similar thymidyl derivative, were used to synthesize four PNAs of the sequence H-GTagAtcACT-NH(CH₂)₂CO₂H, where lower case letters indicate position of a single substitution. The thermal stabilities of the derived duplexes with DNA are found to be dependent on nucleobase and backbone stereochem.

IT 253307-68-5

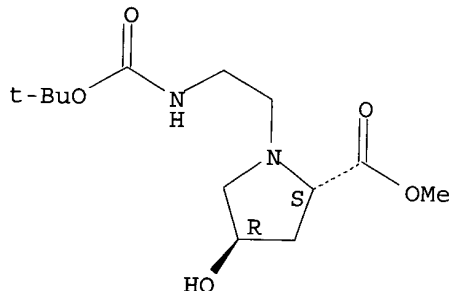
RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation and hybridization studies of mixed base PNAs containing aminoethylprolyl backbone monomers)

RN 253307-68-5 HCAPLUS

CN L-Proline, 1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-4-hydroxy-, methyl ester, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 253307-73-2P 340961-32-2P 340961-33-3P

340961-34-4P 340961-36-6P 340961-46-8P

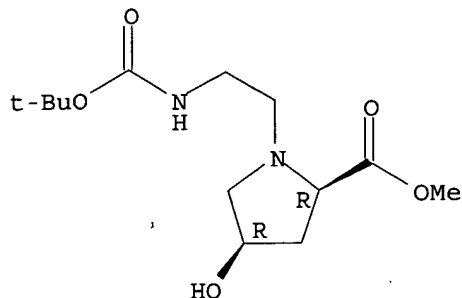
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and hybridization studies of mixed base PNAs containing aminoethylprolyl backbone monomers)

RN 253307-73-2 HCAPLUS

CN D-Proline, 1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-4-hydroxy-, methyl ester, (4R)- (9CI) (CA INDEX NAME)

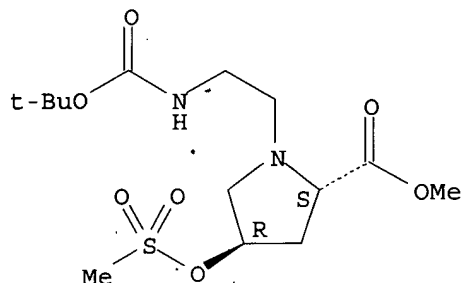
Absolute stereochemistry.



RN 340961-32-2 HCAPLUS

CN L-Proline, 1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-4-[(methylsulfonyl)oxy]-, methyl ester, (4R)-(9CI) (CA INDEX NAME)

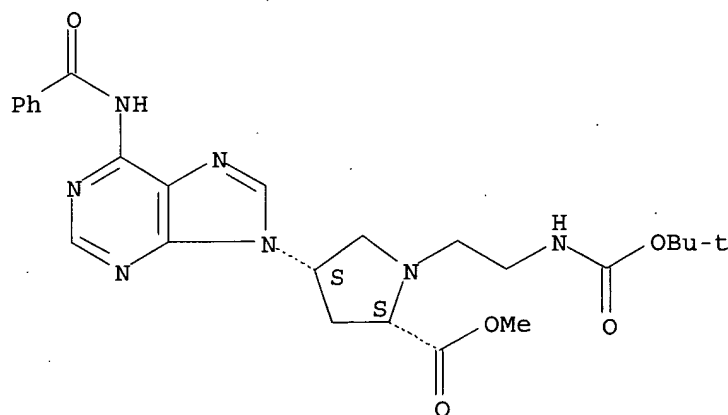
Absolute stereochemistry.



RN 340961-33-3 HCAPLUS

CN L-Proline, 4-[6-(benzoylamino)-9H-purin-9-yl]-1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, methyl ester; (4S)-(9CI) (CA INDEX NAME)

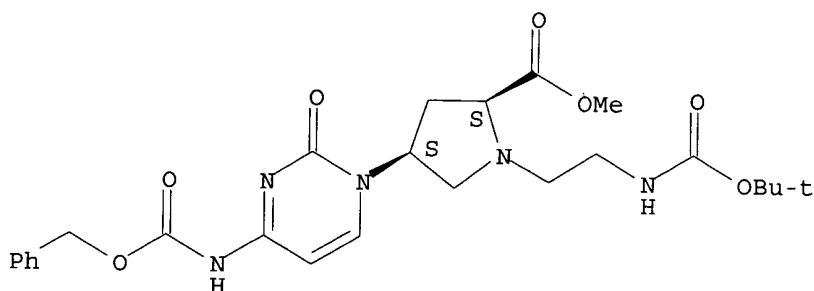
Absolute stereochemistry.



RN 340961-34-4 HCAPLUS

CN L-Proline, 1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-4-[2-oxo-4-[[[(phenylmethoxy)carbonyl]amino]-1(2H)-pyrimidinyl]-, methyl ester, (4S)-(9CI) (CA INDEX NAME)

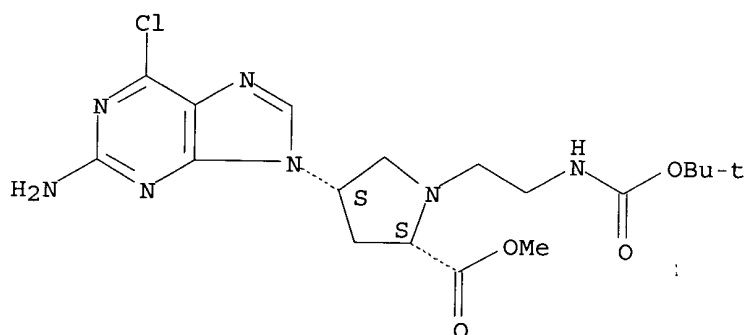
Absolute stereochemistry.



RN 340961-36-6 HCAPLUS

CN L-Proline, 4-(2-amino-6-chloro-9H-purin-9-yl)-1-[2-[[1,1-dimethylethoxy)carbonyl]amino]ethyl]-, methyl ester, (4S)- (9CI) (CA INDEX NAME)

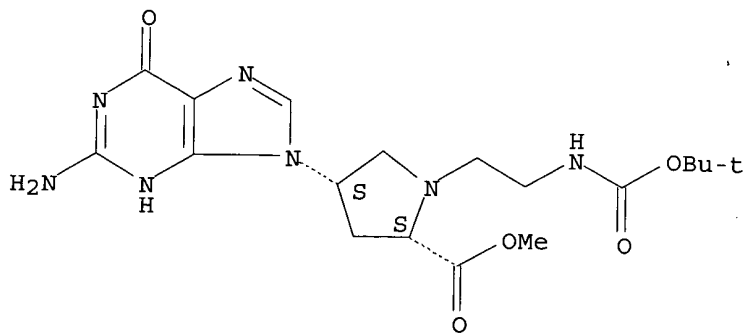
Absolute stereochemistry.



RN 340961-46-8 HCAPLUS

CN L-Proline, 4-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)-1-[2-[[1,1-dimethylethoxy)carbonyl]amino]ethyl]-, methyl ester, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 340961-35-5P 340961-37-7P 340961-38-8P

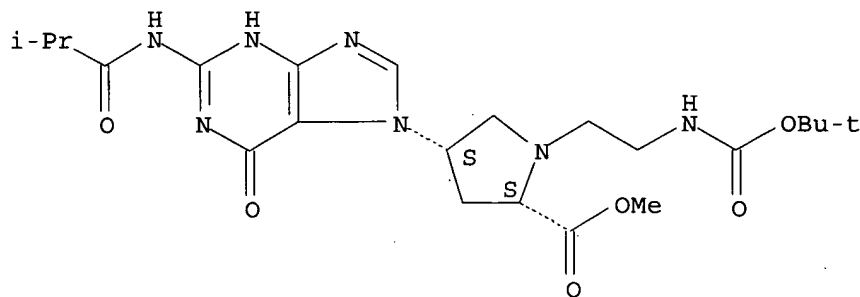
340961-39-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and hybridization studies of mixed base PNAs containing
aminoethylprolyl backbone monomers)

RN 340961-35-5 HCAPLUS

CN L-Proline, 4-[1,6-dihydro-2-[(2-methyl-1-oxopropyl)amino]-6-oxo-7H-purin-7-yl]-1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, methyl ester, (4S)-(9CI) (CA INDEX NAME)

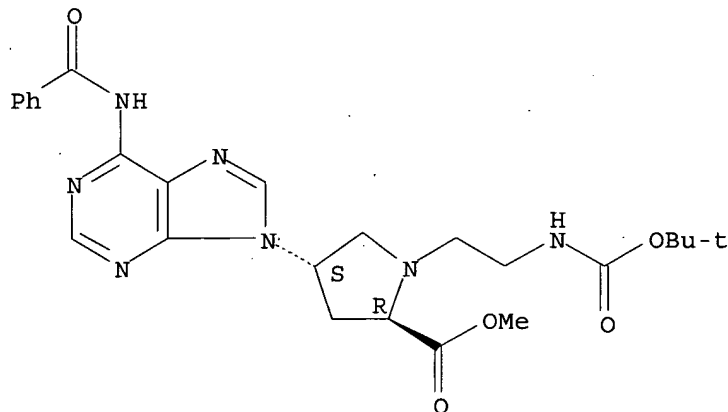
Absolute stereochemistry.



RN 340961-37-7 HCAPLUS

CN D-Proline, 4-[6-(benzoylamino)-9H-purin-9-yl]-1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, methyl ester, (4S)-(9CI) (CA INDEX NAME)

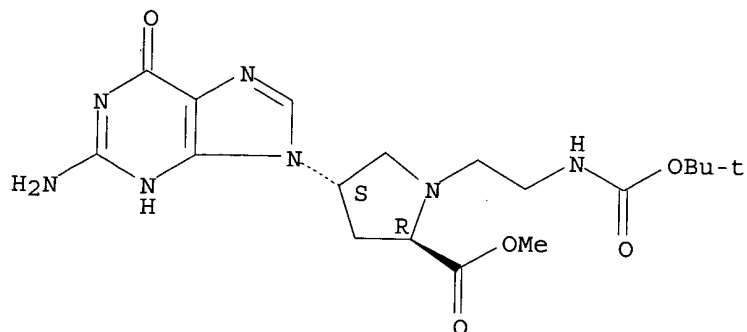
Absolute stereochemistry.



RN 340961-38-8 HCAPLUS

CN D-Proline, 4-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)-1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, methyl ester, (4S)-(9CI) (CA INDEX NAME)

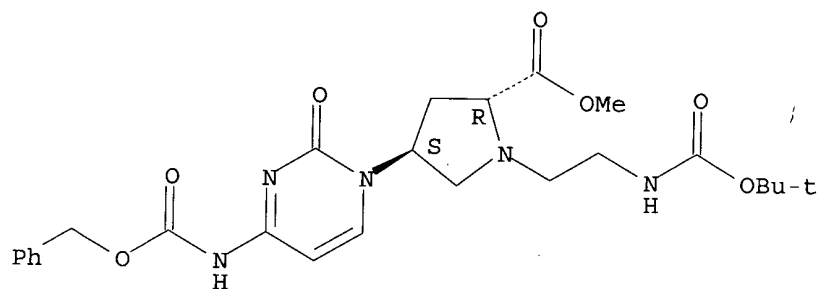
Absolute stereochemistry.



RN 340961-39-9 HCAPLUS

CN D-Proline, 1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-4-[2-oxo-4-[[[phenylmethoxy]carbonyl]amino]-1(2H)-pyrimidinyl]-, methyl ester, (4S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

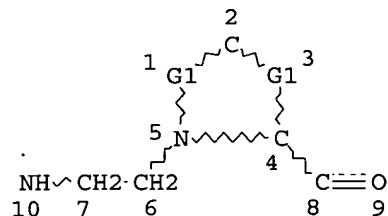
11

THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d que

L11

STR



Claim 22

REP G1=(1-2) CH2

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

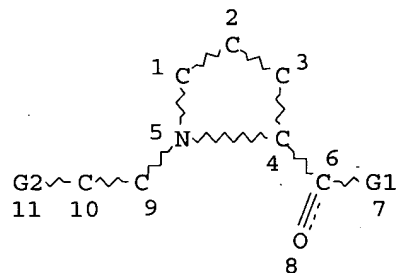
RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 10

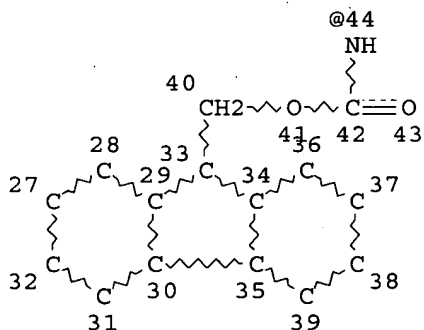
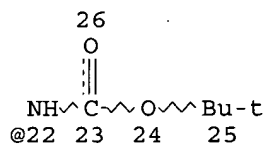
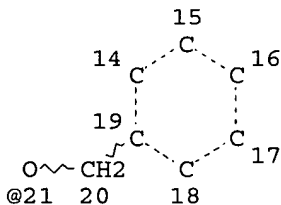
STEREO ATTRIBUTES: NONE

L13 137 SEA FILE=REGISTRY SSS FUL L11

L39 STR



O~Ak
@12 13



VAR G1=H/12/21

VAR G2=NH2/44/22

NODE ATTRIBUTES:

CONNECT IS E1 RC AT 13

DEFAULT MLEVEL IS ATOM

GGCAT IS LOC AT 13

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 44

STEREO ATTRIBUTES: NONE

L40 31 SEA FILE=REGISTRY SUB=L13 SSS FUL L39
L43 7 SEA FILE=REGISTRY ABB=ON PLU=ON L40 AND NCNC3/ES
L45 6 SEA FILE=REGISTRY ABB=ON PLU=ON L43 AND O>5
L46 5 SEA FILE=HCAPLUS ABB=ON PLU=ON L45

=> d l46 ibib abs hitstr 1-5

L46 ANSWER 1 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:347055 HCAPLUS
DOCUMENT NUMBER: 139:80857
TITLE: N7-Guanine as a C+ mimic in hairpin aeg/aepPNA-DNA
triplex: Probing binding selectivity by UV-Tm and
kinetics by fluorescence-based strand-invasion assay
AUTHOR(S): D'Costa, Moneesha; Kumar, Vaijayanti A.; Ganesh,
Krishna N.
CORPORATE SOURCE: Division of Organic Chemistry (Synthesis), National
Chemical Laboratory, Pune, 411008, India
SOURCE: Journal of Organic Chemistry (2003), 68(11), 4439-4445
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:80857

AB N7-substituted guanine (N7G) has been introduced into aminoethylglycyl
bispNA as a C+ mimic to achieve pH-independent triplex formation with
complementary DNA sequences. The introduction of chiral, cationic
aminoethylprolyl units with C+ and C+ mimic N7G in the backbone of bispNAs
influenced the recognition of cDNA in an orientation-selective manner. A
simple fluorescence assay is developed to examine the process of strand
invasion of target DNA duplex by these modified bispNAs and comparative
results of the study employing triplex forming polypyrimidine (C/T) and
purine-pyrimidine mixmer-bispNAs are presented.

IT 340961-34-4P

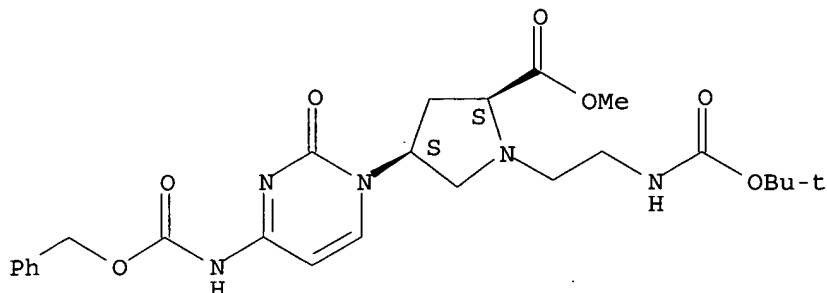
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(N7-guanine as a C+ mimic in hairpin aminoethylglycyl/aminoethylprolylpe
ptide nucleic acid-DNA triplex based on probing binding selectivity by
UV-Tm and kinetics by fluorescence-based strand-invasion assay)

RN 340961-34-4 HCAPLUS

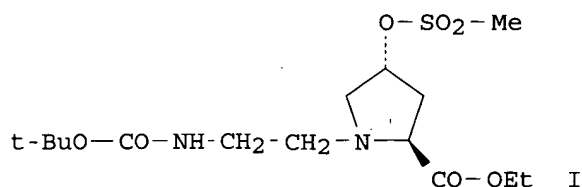
CN L-Proline, 1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-4-[2-oxo-4-
[[[(phenylmethoxy)carbonyl]amino]-1(2H)-pyrimidinyl]-, methyl ester, (4S)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L46 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 2001:710917 HCAPLUS
 DOCUMENT NUMBER: 136:216993
 TITLE: Synthesis and binding affinity of a chiral PNA analogue
 AUTHOR(S): Li, Ying; Jin, Tao; Liu, Keliang
 CORPORATE SOURCE: Beijing Institute of Pharmacology and Toxicology, Beijing, 100850, Peop. Rep. China
 SOURCE: Nucleosides, Nucleotides & Nucleic Acids (2001), 20(9), 1705-1721
 CODEN: MNNAFY; ISSN: 1525-7770
 PUBLISHER: Marcel Dekker, Inc.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB The synthesis of a chiral peptide nucleic acid (PNA), which is composed of N-aminoethyl-cis-4-nucleobase-L-proline units, was described. The chiral PNA monomers containing all four nucleobases (A, T, C and G) were stereoselectively prepared using key intermediate (I), prepared in two steps from (CH3)3COC(O)NH(CH2)2Br and trans-L-hydroxyproline Et ester hydrochloride. The x-ray diffraction data from a single crystal confirmed the configuration of a key intermediate. Binding activity of the oligomers with their complementary DNA targets was also investigated.

IT 386212-13-1P 386212-15-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

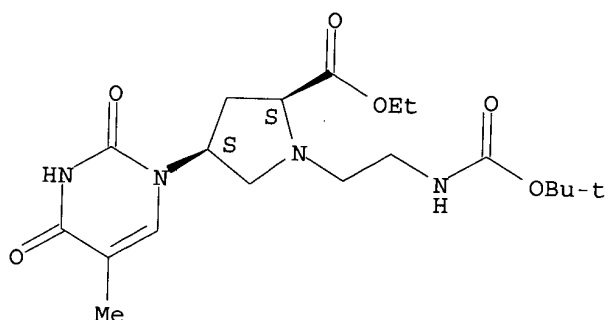
(preparation of cis-L-proline-based PNA oligomers and their hybridization characteristics with DNA)

RN 386212-13-1 HCAPLUS

CN L-Proline, 4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, ethyl ester, (4S)-(9CI)

(CA INDEX NAME)

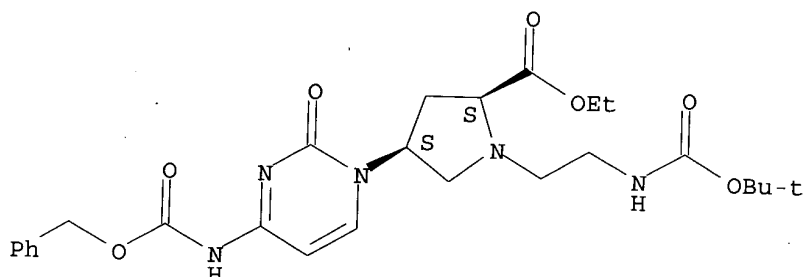
Absolute stereochemistry.



RN 386212-15-3 HCAPLUS

CN L-Proline, 1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-4-[2-oxo-4-[[phenylmethoxy]carbonyl]amino]-1(2H)-pyrimidinyl]-, ethyl ester, (4S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

20

THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L46 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:675176 HCAPLUS

DOCUMENT NUMBER: 135:354283

TITLE: Engineering preferences of hairpin PNA binding to complementary DNA: effect of N7G in aeg/aep PNA backbone

AUTHOR(S): Kumar, V. A.; D'Costa, M.; Ganesh, K. N.

CORPORATE SOURCE: Division of Organic Chemistry (Synthesis), National Chemical Laboratory, Pune, India

SOURCE: Nucleosides, Nucleotides & Nucleic Acids (2001), 20(4-7), 1187-1191

PUBLISHER: CODEN: NNNAFY; ISSN: 1525-7770

DOCUMENT TYPE: Marcel Dekker, Inc.

LANGUAGE: Journal

OTHER SOURCE(S): English

AB Aminoethylglycyl peptide nucleic acid (aegPNA) and aminoethylpropyl

peptide nucleic acid (aepPNA) monomeric units bearing the N7-guanine

nucleobase as a substitute for protonated cytosine (C+) have been shown to bind to a GC base-pair of a duplex in a pH-independent manner when placed in the third strand. The aepPNA backbone exerts a preference for binding in the antiparallel Hoogsteen mode over the parallel Hoogsteen mode.

IT 340961-34-4P

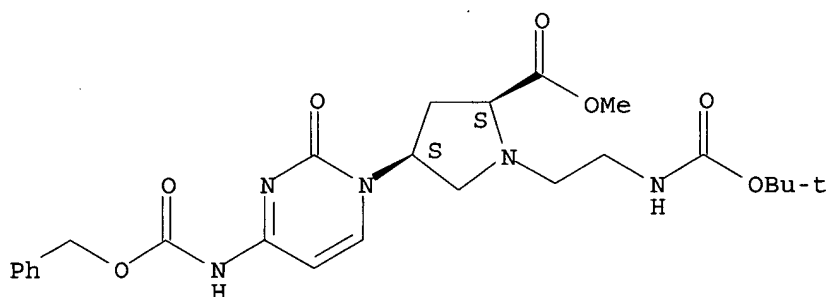
RL: PNU (Preparation, unclassified); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(recognition of DNA is influenced by presence of aminoethylpropyl peptide nucleic acid units in triplex-forming PNA hairpins)

RN 340961-34-4 HCAPLUS

CN L-Proline, 1-[2-[[[(1;1-dimethylethoxy)carbonyl]amino]ethyl]-4-[2-oxo-4-[[[phenylmethoxy)carbonyl]amino]-1(2H)-pyrimidinyl]-, methyl ester, (4S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L46 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:238460 HCAPLUS

DOCUMENT NUMBER: 135:107554

TITLE: Aminoethylprolyl (aep) PNA: Mixed Purine/Pyrimidine Oligomers and Binding Orientation Preferences for PNA:DNA Duplex Formation

AUTHOR(S): D'Costa, Moneesha; Kumar, Vaijayanti; Ganesh, Krishna N.

CORPORATE SOURCE: Division of Organic Chemistry (Synthesis), National Chemical Laboratory, Pune, 411008, India

SOURCE: Organic Letters (2001), 3(9), 1281-1284

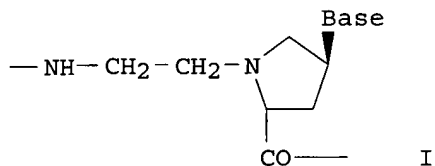
CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB The synthesis of (2S,4S)- and (2R,4S)-aepPNA monomers (I; Base = adenine, guanine, and cytosine) and their incorporation at appropriate positions into aegPNA sequence leads to mixed aeg-aep backbone/mixed nucleobase PNAs. Beginning with (2S,4R)-4-hydroxyl-N-(N-Boc-aminoethyl)-L-proline Me ester (Boc = (CH₃)₃COC(O)-) or its 2R,4R isomer, the hydroxy group was mesylated, and the product reacted with protected Base to give Boc-protected Me esters of I, which, with the similar thymidyl derivative, were used to synthesize four PNAs of the sequence H-GTagAtcACT-NH(CH₂)₂CO₂H, where lower case letters indicate position of a single substitution. The thermal stabilities of the derived duplexes with DNA are found to be dependent on nucleobase and backbone stereochem.

IT **340961-34-4P**

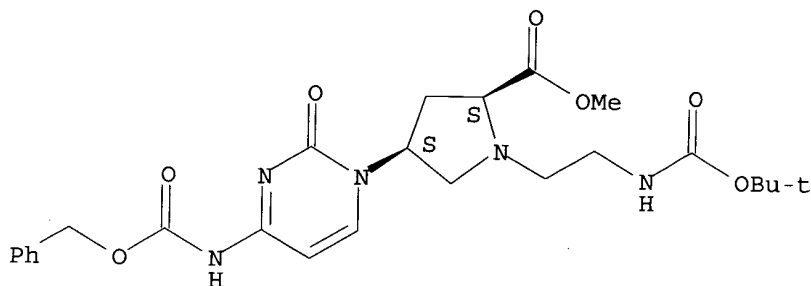
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and hybridization studies of mixed base PNAs containing aminoethylprolyl backbone monomers)

RN 340961-34-4 HCAPLUS

CN L-Proline, 1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-4-[2-oxo-4-[[[(phenylmethoxy)carbonyl]amino]-1(2H)-pyrimidinyl]-, methyl ester, (4S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



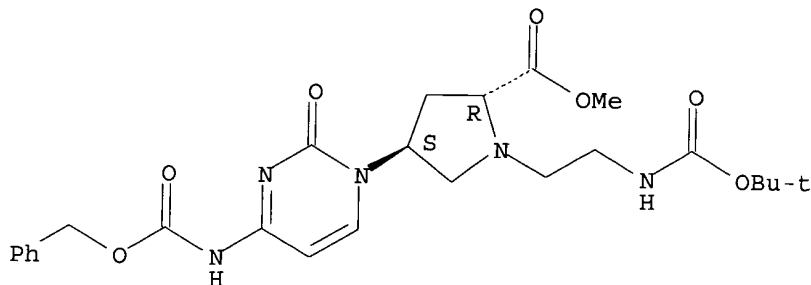
IT **340961-39-9P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and hybridization studies of mixed base PNAs containing aminoethylprolyl backbone monomers)

RN 340961-39-9 HCAPLUS

CN D-Proline, 1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-4-[2-oxo-4-[[[(phenylmethoxy)carbonyl]amino]-1(2H)-pyrimidinyl]-, methyl ester, (4S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L46 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:663052 HCAPLUS

DOCUMENT NUMBER: 132:251401

TITLE: Aminoethylprolyl Peptide Nucleic Acids (aepPNA):
Chiral PNA Analogues That Form Highly Stable
DNA:aepPNA2 Triplexes

AUTHOR(S): D'Costa, Moneesha; Kumar, Vaijayanti A.; Ganesh,
Krishna N.

CORPORATE SOURCE: Division of Organic Chemistry (Synthesis), National
Chemical Laboratory, Pune, 411008, India

SOURCE: Organic Letters (1999), 1(10), 1513-1516
CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The replacement of the glycyl component in the peptide nucleic acid (PNA) backbone by a prolyl unit bearing a nucleobase leads to the aminoethylprolyl (aep) PNAs, which are chiral and cationic. The homo-oligomeric aepPNA binds to complementary DNA sequences with high affinity and sequence specificity, forming highly stable triplexes.

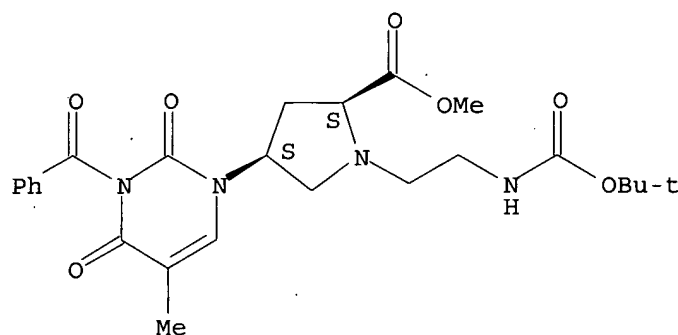
IT 253307-69-6P 253307-74-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of in the synthesis of aminoethylprolyl peptide nucleic acids)

RN 253307-69-6 HCAPLUS

CN L-Proline, 4-(3-benzoyl-3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, methyl ester, (4S)-(9CI) (CA INDEX NAME)

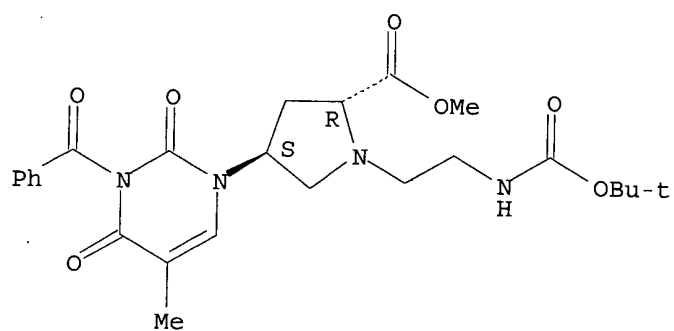
Absolute stereochemistry.



RN 253307-74-3 HCAPLUS

CN D-Proline, 4-(3-benzoyl-3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-1-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, methyl ester, (4S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

22

THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT